ALASKA DEPARTMENT OF ENVIRONMENTAL CONSERVATION

Division of Spill Prevention and Response
Contaminated Sites Program

Procedures for Calculating Cleanup Levels
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Adopted by Reference at 18 AAC 75

Procedures for Calculating Cleanup Levels

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1.0 Introduction

State of Alaska Regulations at 18 AAC 75, Article 3, for Oil and Other Hazardous Substances Pollution Control, govern the cleanup of sites contaminated with oil or other hazardous substances. Sections of this regulation address the selection or development of cleanup levels for contaminated soil and groundwater that are considered protective of human health, safety, and welfare, and the environment. Cleanup levels at a site may be determined by one or more of four methods.

Method one cleanup levels listed in 18 AAC 75.341(a) and (b) apply only to soil contaminated with petroleum hydrocarbons and are not considered risk-based. Method two cleanup levels for approximately 180 chemicals are listed in 18 AAC 75.341(c) and for petroleum hydrocarbons in 18 AAC 75.341(d). These levels are generally risk-based, incorporating toxicity and chemical specific information, assessing multiple routes of exposure in climate settings that reflect the variability found across the state, and the potential for a given chemical to migrate from soil to groundwater. However, if the risk-based cleanup level exceeds the soil saturation or water solubility limit, the cleanup level is set at that limit in compliance with 18 AAC 75.325(f), which requires free product recovery. Though still somewhat generic, the method two levels are considered protective of human exposure for most sites. Determining cleanup levels under method three allows for modification of the default soil cleanup levels to account for site-specific soil and aquifer data or to propose a commercial/industrial exposure scenario. Method four cleanup levels are developed under a risk assessment conducted in accordance with the department's Risk Assessment Procedures Manual (ADEC, 2015).

This document presents the equations used to calculate the default, method two soil cleanup criteria listed in Tables B1 and B2 in 18 AAC 75.341(c) and (d) and groundwater criteria listed in Table C in 18 AAC 75.345(b)(1). The equations presented in Sections 2.0 through 5.0 for individual organic and inorganic chemicals are based on those developed for the Regional Screening Levels (RSLs) by the Oak Ridge National Laboratory under contract to the United States Environmental Protection Agency (EPA), but adapted for Alaska to account for soil and climate variability, and a default cancer risk of 1:100,000.

The equations presented in Section 6.0 for the petroleum fractions are unchanged from the 2008 version of this document. These equations were developed using the 1996 EPA Soil Screening Guidance (U.S. EPA 1996a) and information generated by the Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG, 1997).

Equations are provided for the residential land use scenario only; commercial/industrial land use scenarios must be proposed under a method three (18 AAC 75.340(e)). Procedures for calculating site-specific soil cleanup levels for both Table B1 chemicals and Table B2 petroleum fractions under method three are detailed in Section 7.0.

The standardized default exposure and soil parameters developed by EPA have been used except where noted (See Table 8 for the Standard Default Parameters, found in Appendix B). These exposure parameters are designed to be protective for reasonable maximum exposure (RME)

conditions for long-term/chronic exposures, (U.S. EPA. 1991a; U.S. EPA. 1996a; U.S. EPA. 2002). Chronic oral reference doses (RfD) and chronic inhalation reference concentrations (RfC) are used to calculate non-carcinogenic concentrations. Chronic oral slope factors (CSF_o) are used to evaluate potential human carcinogenic risks. A lifetime cancer risk factor of 1 X 10^{-5} is used, along with a target hazard quotient (THQ) of 1, reported to one significant figure, for noncarcinogens.

For Table B1 and C compounds – equations are presented for non-carcinogenic compounds, carcinogenic compounds, and mutagenic compounds for soil and for groundwater. In addition, for vinyl chloride and trichloroethylene (TCE) in soil and groundwater, a unique set of equations are provided that adjust for early-life cancer risk estimates to derive the cleanup levels.

The groundwater cleanup calculations (Section 2.0) are broken down into equations for ingestion of groundwater, dermal contact with groundwater, and inhalation of volatiles from groundwater. The soil exposure pathway calculations (Section 3.0) are broken down into equations for dermal contact with soil, soil ingestion, and inhalation of volatiles and inhalation of soil particulates using a particulate emission factor (PEF) equation (See Section 5.0, supporting equations). Compounds considered volatile for including the inhalation pathway, are those chemicals with a Henry's Law constant greater than or equal to 1 x 10^{-5} atm-m^3/mole[1] or a vapor pressure greater than or equal to 1 mm Hg.

For the ingestion route, equations use an age-adjusted approach to account for the variation in soil ingestion rates for children depending on age. A number of studies have shown that inadvertent ingestion of soil is common among children six years old and younger (Calabrese et al. 1989, Davis et al. 1990, Van Wijnen et al. 1990). Therefore, the dose method uses an age-adjusted soil ingestion factor that takes into account the difference in daily soil ingestion rates, body weights, and exposure duration for children from 1 to 6 years old and others from 7 to 30 years old. This health-protective approach is chosen to take into account the higher daily rates of soil ingestion in children as well as the longer duration of exposure that is anticipated for a long-term resident. For more on this method, see RAGS Part B (U.S. EPA. 1991a).

The Table B1 method two residential soil cleanup level for the human health pathway provides a single cleanup value that does not exceed a cumulative cancer risk value of 1 X 10^{-5} or a THQ of 1 reported to one significant figure for noncarcinogens for all three soil exposure pathways. Likewise, the Table C groundwater cleanup value is generated by a cumulative risk calculation.

The migration to groundwater criteria for the Table B1 compounds are derived using a soil-water partitioning equation (Section 4.0). This equation back-calculates from the calculated risk-based groundwater cleanup level. A single set of migration to groundwater criteria apply statewide for Table B1, and are based on conservative assumptions about fate and transport mechanisms in the subsurface, accounting for both (1) release of a contaminant in soil leachate and (2) transport of the contaminant through the underlying soil and aquifer to a receptor well (U.S. EPA. 2012).

[1] The atm-m^3/mole units are obtained by multiplying the unitless value by 0.02446 (which comes from multiplying the gas constant (0.0000802 atm-m3/mole-K) by the temperature (298.16 K).

Section 5.0 presents several key equations and factors that support calculations in the proceeding sections, including the approach taken for the dermal absorption route, and derivation of the particulate emission factor, volatilization factor, and other equations.

Equations for the petroleum fraction cleanup values in Table B2 (soil) and Table C (groundwater) are presented in Section 6.0 and, as mentioned above, remain unchanged from the 2008 version of this document. Table B2 petroleum cleanup levels for migration to groundwater are climate-specific, with values established for areas of the state receiving greater than or less than 40 inches of annual precipitation. For all sites with petroleum contamination, the migration to groundwater pathway applies unless the responsible person documents that the pathway is inapplicable, such as in the Arctic zone. Table 1 provides the chemical-specific parameters for the petroleum fractions and Table 2 provides the percentage calculations for combining the aliphatic and aromatic fractions in each range.

Section 7.0 provides procedures for calculating site-specific, method three cleanup levels for the contaminants in both Tables B1 and B2. This includes both the migration-to-groundwater pathway for residential land use scenarios, and also for the commercial/industrial exposure pathways. Tables 3 through 5 list the parameters that can be modified with site-specific data for both Table B1 and B2 compounds.

Table 6 and Table 7 in Appendix A provides the toxicity and chemical-specific parameters for the organic and inorganic chemicals in Table B1 and C. These values are selected from several different references, using the following hierarchy:

- Toxicity
    - EPA's Integrated Risk Information System (IRIS)
    - Professional Peer-Reviewed Toxicity Value (PPRTV)
    - Other toxicity values
        - Agency for Toxic Substances and Disease Registry (ATSDR) Minimal Risk Level (MRLs)
        - California Environmental Protection Agency (Cal EPA) criteria
        - Other sources
- Organic Carbon Partition Coefficient (Koc) (L/kg)
    - Estimation Programs Interface (EPI) Suite estimated values
    - EPA Soil Screening Level (SSL) Exhibit C-1
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds. Knovel, 2003 estimated values
    - EPI Suite experimental values
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds. Knovel, 2003 experimental values
- Dermal Permeability Coefficient (Kp) (cm/hour)
    - EPI Suite estimated values
    - RAGS Part E.
- Effective Predictive Domain (EPD)
    - Calculated based on RAGS Part E criteria for MW and log Kow.
- Fraction Absorbed (FA)
    - RAGS Part E Exhibit B-3; Calculated.

- Molecular Weight (MW) (g/mole)
    - Syracuse Research Corporation (SRC). 2005. PHYSPROP Database. SRC. Syracuse, NY. Accessed July 2005.
    - EPI Suite
    - CRC Handbook of Chemistry and Physics
    - Perry's Chemical Engineers' Handbook (Various Editions).McGraw-Hill
    - Lange's Handbook of Chemistry (Various Editions)
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds
- Water Solubility (S) (mg/L at 25 °C, unless otherwise stated in the source.).
    - SRC PHYSPROP
    - EPI experimental values
    - CRC Handbook of Chemistry and Physics
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds experimental values
    - Perry's Chemical Engineers' Handbook (Various Editions).McGraw-Hill
    - Lange's Handbook of Chemistry (Various Editions)
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds estimated values
    - EPI estimated values
- Unitless Henry's Law Constant (H' at 25 °C, unless otherwise stated in the source.)
    - SRC PHYSPROP
    - EPI experimental values
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds experimental values
    - EPI Suite group-estimated values
    - EPI Suite bond-estimated values
- Henry's Law Constant (atm-m3/mole at 25 °C, unless otherwise stated in the source.)
    - SRC PHYSPROP
    - EPI experimental values
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds experimental values
    - EPI group-estimated values
    - EPI bond-estimated values
- Diffusivity in Air (Dia) (cm2/s)
    - EPA's WATER9 equations.
- Diffusivity in Water (Diw) (cm2/s)
    - EPA's WATER9 equations.
- Soil-Water Partition Coefficient (Kd) (cm3/g).
    - SSL
    - Baes, C.F. 1984. Oak Ridge National Laboratory. A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides through Agriculture
- Density (g/cm3)
    - CRC Handbook of Chemistry and Physics
    - Perry's Chemical Engineers' Handbook (Various Editions).McGraw-Hill

    - Lange's Handbook of Chemistry (Various Editions)
    - IRIS.
- Melting Point (MP °C)
    - SRC PHYSPROP
    - EPI experimental values
    - CRC Handbook of Chemistry and Physics
    - Perry's Chemical Engineers' Handbook (Various Editions).McGraw-Hill
    - Lange's Handbook of Chemistry (Various Editions)
    - EPI Suite estimated values
- log Octanol-Water Partition Coefficient (log Kow)
    - EPI experimental values
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds experimental values
    - EPI Suite estimated values
    - Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds estimated values

Table 8 provides the list of Standard Default Parameters used in the equations in this document and calculations via which the Table B1 cleanup levels are derived.

2.0 Groundwater Cleanup Level Equations

2.1 Groundwater Cleanup Level Equation for Non-Carcinogenic Compounds

Cleanup level equations for exposure to non-carcinogenic compounds in groundwater are presented below. The terms used in the equations are defined in Appendix B. The equations include exposure routes via ingestion, dermal contact, and inhalation of volatiles, which are then totaled to produce a final value.

2.1.1 Ingestion of Water

$$\mathrm{CL_{water-nc-ing}(\mu g/L)} = \frac{\mathrm{THQ} \times \mathrm{AT_{reswc}}\left(\frac{365\ \mathrm{days}}{\mathrm{year}} \times \mathrm{ED_{reswc}}(6\ \mathrm{years})\right) \times \mathrm{BW_{reswc}}(15\ \mathrm{kg}) \times \left(\frac{1000\mu g}{\mathrm{mg}}\right)}{\mathrm{EF_{reswc}}\left(350\frac{\mathrm{days}}{\mathrm{year}}\right) \times \mathrm{ED_{reswc}}(6\ \mathrm{years}) \times \frac{1}{\mathrm{RfD_0}\left(\frac{\mathrm{mg}}{\mathrm{kg\cdot d}}\right)} \times \mathrm{IRW_{reswc}}\left(0.78\frac{\mathrm{L}}{\mathrm{day}}\right)}$$

2.1.2 Dermal for Inorganics

$$\mathrm{CL_{water-nc-der}(\mu g/L)} = \frac{\mathrm{DA_{event}}\left(\frac{\mu g}{\mathrm{cm^2\cdot\ event}}\right) \times \left(\frac{1000\mathrm{cm}^3}{\mathrm{L}}\right)}{\mathrm{K_p}\left(\frac{\mathrm{cm}}{\mathrm{hr}}\right) \times ET_{reswc}^{der}\left(0.54\ \frac{hours}{event}\right)}$$

Where:

$$DA_{event}\left(\frac{\mu g}{cm^2 \cdot event}\right) = \frac{THQ \times AT_{reswc}\left(\frac{365\ days}{year} \times ED_{reswc}(6\ years)\right) \times \left(\frac{1000\mu g}{mg}\right) \times BW_{reswc}(15\ kg)}{\left(\frac{1}{RfD_0\left(\frac{mg}{kg \cdot day}\right) \times GIABS}\right) \times EV_{reswc}\left(\frac{1\ events}{day}\right) \times ED_{reswc}(6\ years) \times EF_{reswc}\left(\frac{350\ days}{year}\right) \times SA_{reswc}(6{,}378\ cm^2)}$$

2.1.3 Dermal for Organics

$$\text{If } ET_{reswc}^{der}\left(0.54\ \frac{hours}{event}\right) \leq \mathrm{t^*(hr)}, \text{ then } \mathrm{CL_{water-nc-der}(\mu g/L)} = \frac{\mathrm{DA_{event}}\left(\frac{\mu g}{\mathrm{cm^2\cdot\ event}}\right) \times \left(\frac{1000\mathrm{cm}^3}{\mathrm{L}}\right)}{2\ \times \mathrm{FA} \times \mathrm{K_p}\left(\frac{\mathrm{cm}}{\mathrm{hr}}\right)\sqrt{\frac{6 \times \tau_{\mathrm{event}}\left(\frac{\mathrm{hours}}{\mathrm{event}}\right) \times \text{If } ET_{reswc}^{der}\left(0.54\ \frac{hours}{event}\right)}{\pi}}}$$

Or,

$$\text{If } ET_{reswc}^{der}\left(0.54\ \frac{hours}{event}\right) > \text{t}^{*}(\text{hr}), \text{then } \text{CL}_{\text{water-nc-der}}(\mu\text{g/L}) = \frac{\text{DA}_{\text{event}}\left(\frac{\mu\text{g}}{\text{cm}^2\cdot\text{event}}\right)\times\left(\frac{1000\text{cm}^3}{\text{L}}\right)}{\text{FA}\times\text{K}_\text{p}\left(\frac{\text{cm}}{\text{hr}}\right)\left[\frac{ET_{reswc}^{der}\left(0.54\frac{hours}{event}\right)}{1+\text{B}}+2\times\tau_{\text{event}}\left(\frac{\text{hours}}{\text{event}}\right)\times\left(\frac{1+3\text{B}+3\text{B}^2}{(1+\text{B})^2}\right)\right]}$$

2.1.4 Inhalation of Volatiles

$$\text{CL}_{\text{water-nc-inh}}(\mu\text{g/L}) = \frac{\text{THQ}\times\text{AT}_{\text{reswc}}\left(\frac{365\text{ days}}{\text{year}}\times\text{ED}_{\text{reswc}}(6\text{ years})\right)\times\left(\frac{1000\mu\text{g}}{\text{mg}}\right)}{\text{EF}_{\text{reswc}}\left(350\ \frac{\text{days}}{\text{year}}\right)\times\text{ED}_{\text{reswc}}(6\text{ years})\times ET_{reswc}^{inh}\left(\frac{24\text{ hours}}{\text{day}}\right)\times\left(\frac{1\text{ day}}{24\text{ hours}}\right)\times\frac{1}{\text{RfC}\left(\frac{\text{mg}}{\text{m}^3}\right)}\times\text{K}\ \left(\frac{0.5\text{L}}{\text{m}^3}\right)}$$

2.1.5 Total Non-carcinogenic Risk for All Groundwater Exposure Pathways

$$CL_{res-water-nc-tot}\left(\frac{\mu g}{L}\right) = \frac{1}{\frac{1}{CL_{water-nc-ing}}+\frac{1}{CL_{water-nc-der}}+\frac{1}{CL_{water-nc-inh}}}$$

2.2 Groundwater Cleanup Level Equation for Carcinogenic Compounds

Cleanup level equations for exposure to carcinogenic compounds in groundwater are presented below. The equations include exposure routes via ingestion, dermal contact, and inhalation of volatiles, which are then totaled to produce a final value.

2.2.1 Ingestion of Water

$$CL_{water-ca-ing}(\mu g/L) = \frac{TR\times AT_{resw}\left(\frac{365\ days}{year}\times LT(70\ years)\right)\times\left(\frac{1000\mu g}{mg}\right)}{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1}\times\left(IFW_{res-adj}\left(327.95\frac{L}{kg}\right)\right)}$$

Where:

$$IFW_{res-adj}\left(327.95\frac{L}{Kg}\right) = \frac{ED_{reswc}(6\ years)\times EF_{reswc}\left(350\frac{days}{year}\right)\times IRW_{reswc}\left(0.78\frac{L}{day}\right)}{BW_{reswc}(15\ kg)} + \frac{[ED_{resw}(26\ years)-ED_{reswc}(6\ years)]\times EF_{reswa}\left(350\frac{days}{year}\right)\times IRW_{reswa}\left(2.5\frac{L}{day}\right)}{BW_{reswa}(80\ kg)}$$

2.2.2 Dermal for Inorganics

$$CL_{water-ca-der}(\mu g/L) = \frac{DA_{event}\left(\frac{\mu g}{cm^2 \cdot event}\right) \times \left(\frac{1000 cm^3}{L}\right)}{K_p\left(\frac{cm}{hr}\right) \times ET^{der}_{resw-adj}\left(0.67077 \frac{hours}{event}\right)}$$

2.2.3 Dermal for Organics

$$IF\ ET^{der}_{resw-adj}\left(0.67077 \frac{hours}{event}\right) \leq t^*(hr), then\ CL_{water-ca-der}(\mu g/L) = \frac{DA_{event}\left(\frac{\mu g}{cm^2 \cdot event}\right) \times \left(\frac{1000 cm^3}{L}\right)}{2 \times FA \times K_p\left(\frac{cm}{hr}\right)\sqrt{\frac{6 \times \tau_{event}\left(\frac{hours}{event}\right) \times ET^{der}_{resw-adj}\left(0.67077 \frac{hours}{event}\right)}{\pi}}}$$

Or,

$$IF\ ET^{der}_{resw-adj}\left(0.67077 \frac{hours}{event}\right) > t^*(hr), then\ CL_{water-ca-der}(\mu g/L) = \frac{DA_{event}\left(\frac{\mu g}{cm^2 \cdot event}\right) \times \left(\frac{1000\ cm^3}{L}\right)}{FA \times K_p\left(\frac{cm}{hr}\right) \times \left[\frac{ET_{resw-adj}\left(0.67077 \frac{hours}{event}\right)}{1+B} + 2 \times \tau_{event}\left(\frac{hours}{event}\right) \times \left(\frac{1+3B+3B^2}{(1+B)^2}\right)\right]}$$

Where:

$$DA_{event}\left(\frac{\mu g}{cm^2 \cdot event}\right) = \frac{TR \times AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right) \times \left(\frac{1000 \mu g}{mg}\right)}{\left(\frac{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1}}{GIABS}\right) \times DFW_{res-adj}\left(2721670 \frac{cm^2 \cdot event}{kg}\right)}$$

$$DFW_{res-adj}\left(2721670 \frac{cm^2 \cdot event}{kg}\right) = \frac{EV_{reswc}\left(\frac{1\ events}{day}\right) \times ED_{reswc}(6\ years) \times EF_{reswc}\left(350 \frac{days}{year}\right) \times SA_{reswc}(6{,}378\ cm^2)}{BW_{reswc}(15\ kg)} + \frac{EV_{reswa}\left(\frac{1\ events}{day}\right) \times ED_{reswa}(20\ years) \times EF_{reswa}\left(350 \frac{days}{year}\right) \times SA_{reswa}(20{,}900\ cm^2)}{BW_{reswa}(80 kg)}$$

And:

$$ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right) = \frac{ET^{der}_{reswc}\left(0.54\,\frac{hours}{event}\right) \times ED_{reswc}(6\ years) + ET^{der}_{reswa}\left(0.71\,\frac{hours}{event}\right) \times [ED_{resw}(26\ years) - ED_{reswc}(6\ years)]}{ED_{resw}(26\ years)}$$

2.2.4 Inhalation of Volatiles

$$CL_{water-ca-inh}(\mu g/L) = \frac{TR \times AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{EF_{resw}\left(\frac{350\ days}{year}\right) \times ED_{resw}(26\ years) \times ET^{inh}_{resw}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times K\left(\frac{0.5L}{m^3}\right)}$$

2.2.5 Total Carcinogenic Risk for All Groundwater Exposure Pathways

$$CL_{water-ca-tot}(\mu g/L) = \frac{1}{\frac{1}{CL_{water-ca-ing}} + \frac{1}{CL_{water-ca-der}} + \frac{1}{CL_{water-ca-inh}}}$$

2.3 Mutagenic Equation for Groundwater

Cleanup level equations for exposure to mutagenic compounds in groundwater are presented below. The equations include exposure routes via ingestion, dermal contact, and inhalation of volatiles, which are then totaled to produce a final value.

2.3.1 Ingestion of Water

$$CL_{water-mu-ing}(\mu g/L) = \frac{TR \times AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right) \times \left(\frac{1000\ \mu g}{mg}\right)}{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1} \times IFWM_{res-adj}\left(1019.9\,\frac{L}{kg}\right)}$$

Where:

$$IFWM_{res-adj}\left(1019.9\frac{L}{Kg}\right) = \frac{ED_{0-2}(2\ years)\times EF_{0-2}\left(350\frac{days}{year}\right)\times IRW_{0-2}\left(0.78\frac{L}{day}\right)\times 10}{BW_{0-2}(15\ kg)} + \frac{ED_{2-6}(4\ years)\times EF_{2-6}\left(350\frac{days}{year}\right)\times IRW_{2-6}\left(0.78\frac{L}{day}\right)\times 3}{BW_{2-6}(15\ kg)} + \frac{ED_{6-16}(10\ years)\times EF_{6-16}\left(350\frac{days}{year}\right)\times IRW_{6-16}\left(2.5\frac{L}{day}\right)\times 3}{BW_{6-16}(80\ kg)} + \frac{ED_{16-60}(10\ years)\times EF_{16-30}\left(350\frac{days}{year}\right)\times IRW_{16-30}\left(2.5\frac{L}{day}\right)\times 1}{BW_{16-30}(80\ kg)}$$

2.3.2 Dermal

2.3.2.1 Dermal for Inorganics:

$$CL_{water-mu-der}(\mu g/L) = \frac{DA_{event}\left(\frac{\mu g}{cm^2\cdot event}\right)\times\left(\frac{1000cm^3}{L}\right)}{K_p\left(\frac{cm}{hr}\right)\times ET_{resw-madj}\left(0.67077\frac{hours}{event}\right)}$$

2.3.2.2 Dermal for Organics:

$$IF\ ET_{resw-madj}\left(0.67077\frac{hours}{event}\right)\le t^*(hr), then\ CL_{water-mu-der}(\mu g/L) = \frac{DA_{event}\left(\frac{\mu g}{cm^2\cdot event}\right)\times\left(\frac{1000cm^3}{L}\right)}{2\times FA\times K_p\left(\frac{cm}{hr}\right)\sqrt{\frac{6\times\tau_{event}\left(\frac{hours}{event}\right)\times ET_{resw-madj}\left(0.67077\frac{hours}{event}\right)}{\pi}}}$$

Or

$$IF\ ET_{resw-madj}\left(0.67077\frac{hours}{event}\right) > t^*(hr), then\ CL_{water-mu-der}(\mu g/L) = \frac{DA_{event}\left(\frac{\mu g}{cm^2\cdot event}\right)\times\left(\frac{1000cm^3}{L}\right)}{FA\times K_p\left(\frac{cm}{hr}\right)\times\left[\frac{ET_{resw-madj}\left(0.67077\frac{hours}{event}\right)}{1+B}+2\times\tau_{event}\left(\frac{hours}{event}\right)\times\left(\frac{1+3B+3B^2}{(1+B)^2}\right)\right]}$$

Where:

$$DA_{event}\left(\frac{\mu g}{cm^2 \cdot event}\right) = \frac{TR \times AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right) \times \left(\frac{1000 \mu g}{mg}\right)}{\left(\frac{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1}}{GIABS}\right) \times DFWM_{res-adj}\left(8419740 \frac{events \cdot cm^2}{kg}\right)}$$

Where:

$$DFWM_{res-adj}\left(8419740 \frac{events \cdot cm^2}{kg}\right) = \left[\left(\frac{EV_{0-2}\left(\frac{1\ events}{day}\right) \times ED_{0-2}(2\ years) \times EF_{0-2}\left(350 \frac{days}{year}\right) \times SA_{0-2}(6{,}378\ cm^2) \times 10}{BW_{0-2}(15\ kg)}\right) + \left(\frac{EV_{2-6}\left(\frac{1\ events}{day}\right) \times ED_{2-6}(4\ years) \times EF_{2-6}\left(350 \frac{days}{year}\right) \times SA_{2-6}(6{,}378\ cm^2) \times 3}{BW_{2-6}(15\ kg)}\right) + \left(\frac{EV_{6-16}\left(\frac{1\ events}{day}\right) \times ED_{6-16}(10\ years) \times EF_{6-16}\left(350 \frac{days}{year}\right) \times SA_{6-16}(20{,}900\ cm^2) \times 3}{BW_{6-16}(80\ kg)}\right) + \left(\frac{EV_{16-26}\left(\frac{1\ events}{day}\right) \times ED_{16-26}(10\ years) \times EF_{16-26}\left(350 \frac{days}{year}\right) \times SA_{16-26}(20{,}900\ cm^2) \times 1}{BW_{16-26}(80\ kg)}\right)\right]$$

And:

$$ET_{resw-madj}\left(0.67077 \frac{hours}{event}\right) = \frac{\begin{pmatrix} ET_{0-2}^{der}\left(0.54 \frac{hours}{event}\right) \times ED_{0-2}(2\ years) + ET_{2-6}^{der}\left(0.54 \frac{hour}{event}\right) \times ED_{2-6}(4\ years) \\ +ET_{6-16}^{der}\left(0.71 \frac{hours}{event}\right) \times ED_{6-16}(10\ years) + ET_{16-26}^{der}\left(0.71 \frac{hours}{event}\right) \times ED_{16-30}(10\ years) \end{pmatrix}}{ED_{0-2}(2\ years) + ED_{2-6}(4\ years) + ED_{6-16}(10\ years) + ED_{16-26}(10\ years)}$$

2.3.3 Inhalation of Volatiles

$$CL_{water-mu-inh}(\mu g/L) = \frac{TR \times AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{K\left(\frac{0.5L}{m^3}\right) \times ET_{resw}^{inh}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times \left[\begin{pmatrix} \left(ED_{0-2}(years) \times EF_{0-2}\left(350\ \frac{days}{year}\right) \times IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times 10\right) + \left(ED_{2-6}(years) \times EF_{2-6}\left(350\ \frac{days}{year}\right) \times IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times 3\right) + \\ \left(ED_{6-16}(years) \times EF_{6-10}\left(350\ \frac{days}{year}\right) \times IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times 3\right) + \left(ED_{16-26}(years) \times EF_{16-26}\left(350\ \frac{days}{year}\right) \times IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times 1\right) \end{pmatrix}\right]}$$

2.3.4 Total Mutagenic Risk for All Groundwater Exposure Pathways

$$CL_{water-mu-tot}(\mu g/L) = \frac{1}{\frac{1}{CL_{water-mu-ing}} + \frac{1}{CL_{water-mu-der}} + \frac{1}{CL_{water-mu-inh}}}$$

2.4 Vinyl Chloride

2.4.1 Ingestion of Water

$$CL_{water-vc-ing}(\mu g/L) = \frac{TR}{\frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1} \times IFW_{res-adj}\left(327.95\frac{L}{kg}\right) \times \frac{mg}{1000\mu g}}{AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right)} + \frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1} \times IRW_{reswc}\left(0.78\frac{L}{day}\right) \times \frac{mg}{1000\mu g}}{BW_{reswc}(15\text{kg})}}$$

Where:

$$IFW_{res-adj}\left(327.95\frac{L}{kg}\right) = \frac{ED_{reswc}(6\ years) \times EF_{reswc}\left(350\frac{days}{year}\right) \times IRW_{reswc}\left(0.78\frac{L}{day}\right)}{BW_{reswc}(15\ Kg)} + \frac{[ED_{resw}(26\ years) - ED_{reswc}(6\ years)] \times EF_{reswa}\left(350\frac{days}{year}\right) \times IRW_{reswa}\left(2.5\frac{L}{day}\right)}{BW_{reswa}(80\ kg)}$$

2.4.2 Dermal

$$IF\ ET^{der}_{resw-adj}\left(0.67077\frac{hours}{event}\right) \leq t^*(hr), then\ CL_{water-vc-der}(\mu g/L) = \frac{DA_{event}\left(\frac{\mu g}{cm^2\cdot event}\right) \times \left(\frac{1000cm^3}{L}\right)}{2 \times FA \times K_p\left(\frac{cm}{hr}\right)\sqrt{\frac{6 \times \tau_{event}\left(\frac{hours}{event}\right) \times ET^{der}_{resw-adj}\left(0.67077\frac{hours}{event}\right)}{\pi}}}$$

Or,

$$IF\ ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right) > t^{*}(hr), then\ CL_{water-\mathrm{vc}-der}(\mu g/L)$$
$$= \frac{DA_{event}\left(\frac{\mu g}{cm^2\cdot\ event}\right)\times\left(\frac{1000\ cm^3}{L}\right)}{FA\times K_p\left(\frac{cm}{hr}\right)\times\left[\frac{ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right)}{1+B}+2\times\tau_{event}\left(\frac{hours}{event}\right)\times\left(\frac{1+3B+3B^2}{(1+B)^2}\right)\right]}$$

Where:

$$DA_{event}\left(\frac{\mu g}{cm^2\cdot event}\right) = \frac{TR}{\left(\frac{\left(\frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1}}{GIABS}\right)\times DFW_{res-adj}\left(2721670\,\frac{cm^2\cdot event}{kg}\right)}{AT_{resw}\left(\frac{365\ days}{year}\times \mathrm{LT}(70\ \mathrm{years})\right)\times\frac{1000\,\mu g}{mg}}\right)+\left(\frac{\left(\frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1}}{GIABS}\right)\times EV_{reswc}\left(\frac{1\ event}{day}\right)\times SA_{reswc}(6378\ cm^2)}{BW_{reswc}(15kg)\times\frac{1000\,\mu g}{mg}}\right)}$$

Where:

$$DFW_{res-adj}\left(2721670\,\frac{cm^2\cdot event}{kg}\right) = \frac{EV_{reswc}\left(\frac{1\ events}{day}\right)\times ED_{reswc}(6\ years)\times EF_{reswc}\left(350\,\frac{days}{year}\right)\times SA_{reswc}(6{,}378\ cm^2)}{BW_{reswc}(15\ kg)} + \frac{EV_{reswa}\left(\frac{1\ events}{day}\right)\times ED_{reswa}(24\ years)\times EF_{reswa}\left(350\,\frac{days}{year}\right)\times SA_{reswa}(20{,}900\ cm^2)}{BW_{reswa}(80kg)}$$

And:

$$ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right) = \frac{ET^{der}_{reswc}\left(0.54\,\frac{hours}{event}\right)\times ED_{reswc}(6\ years)+ET^{der}_{reswa}\left(0.71\,\frac{hours}{event}\right)\times[ED_{resw}(26\ years)-ED_{reswc}(6\ years)]}{ED_{resw}(26\ years)}$$

2.4.3 Inhalation

$$CL_{water-vc-inh}(\mu g/L) = \frac{TR}{\left(\frac{IUR\left(\frac{\mu g}{m^3}\right)^{-1}\times EF_{resw}\left(\frac{350\ days}{year}\right)\times ED_{resw}(26\ years)\times ET^{inh}_{resw}\left(\frac{24\ hours}{day}\right)\times\left(\frac{1\ day}{24\ hours}\right)\times K\left(\frac{0.5L}{m^3}\right)}{AT_{resw}\left(\frac{365\ days}{year}\times LT(70\ years)\right)}\right)+\left(IUR\left(\frac{\mu g}{m^3}\right)^{-1}\times K\left(\frac{0.5L}{m^3}\right)\right)}$$

2.4.4 Total

$$CL_{water-vc-tot}(mg/kg) = \frac{1}{\frac{1}{CL_{water-vc-ing}} + \frac{1}{CL_{water-vc-der}} + \frac{1}{CL_{water-vc-inh}}}$$

2.5 Trichloroethylene

2.5.1 Ingestion of Water

$$CL_{water-tce-ing}(\mu g/L) = \frac{TR \times AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right) \times \frac{(1000 \mu g)}{mg}}{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1} \times \left[\left(CAF_0(0.804) \times IFW_{resw-adj}\left(327.95 \frac{L}{kg}\right)\right) + \left(MAF_0(0.202) \times IFWM_{res-adj}\left(1019.9 \frac{L}{kg}\right)\right)\right]}$$

Where:

$$CAF_O(0.804) = \frac{CSF_O\left(0.037 \frac{mg}{kg \cdot day}\right)^{-1}\ NHL + Liver\ Oral\ Slope\ Factor}{CSF_O\left(0.046 \frac{mg}{kg \cdot day}\right)^{-1}\ Adult - Based\ Oral\ Slope\ Factor}$$

$$MAF_O(0.202) = \frac{CSF_O\left(0.0093 \frac{mg}{kg \cdot day}\right)^{-1}\ Kidney\ Oral\ Slope\ Factor}{CSF_O\left(0.046 \frac{mg}{kg \cdot day}\right)^{-1}\ Adult - Based\ Oral\ Slope\ Factor}$$

$$IFW_{res-adj}\left(327.95 \frac{L}{kg}\right) = \frac{ED_{reswc}(6\ years) \times EF_{reswc}\left(350 \frac{days}{year}\right) \times IRW_{reswc}\left(0.78 \frac{L}{day}\right)}{BW_{reswc}(15\ kg)} + \frac{[ED_{resw}(26\ years) - ED_{reswc}(6\ years)] \times EF_{reswa}\left(350 \frac{days}{year}\right) \times IRW_{reswa}\left(2.5 \frac{L}{day}\right)}{BW_{reswa}(80\ kg)}$$

$$IFWM_{res-adj}\left(1019.9 \frac{L}{Kg}\right) = \frac{ED_{0-2}(2\ years) \times EF_{0-2}\left(350 \frac{days}{year}\right) \times IRW_{0-2}\left(0.78 \frac{L}{day}\right) \times 10}{BW_{0-2}(15\ kg)} + \frac{ED_{2-6}(4\ years) \times EF_{2-6}\left(350 \frac{days}{year}\right) \times IRW_{2-6}\left(0.78 \frac{L}{day}\right) \times 3}{BW_{2-6}(15\ kg)} + \frac{ED_{6-16}(10\ years) \times EF_{6-16}\left(350 \frac{days}{year}\right) \times IRW_{6-16}\left(2.5 \frac{L}{day}\right) \times 3}{BW_{6-16}(80\ kg)} + \frac{ED_{16-26}(10\ years) \times EF_{16-26}\left(350 \frac{days}{year}\right) \times IRW_{16-26}\left(2.5 \frac{L}{day}\right) \times 1}{BW_{16-26}(80\ kg)}$$

2.5.2 Dermal

$$IF\ ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right) \le t^{*}(hr), then\ CL_{water-tce-der}(\mu g/L)$$

$$= \frac{DA_{tce-event}\left(\frac{\mu g}{cm^2 \cdot event}\right) \times \left(\frac{1000 cm^3}{L}\right)}{2 \times FA \times K_p\left(\frac{cm}{hr}\right)\sqrt{\frac{6 \times \tau_{event}\left(\frac{hours}{event}\right) \times ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right)}{\pi}}}$$

Or,

$$IF\ ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right) > t^{*}(hr), then\ CL_{water-tce-der}(\mu g/L)$$

$$= \frac{DA_{tce-event}\left(\frac{\mu g}{cm^2 \cdot\ event}\right) \times \left(\frac{1000\ cm^3}{L}\right)}{FA \times K_p\left(\frac{cm}{hr}\right) \times \left[\frac{ET^{der}_{resw-adj}\left(0.67077\,\frac{hours}{event}\right)}{1+B} + 2 \times \tau_{event}\left(\frac{hours}{event}\right) \times \left(\frac{1+3B+3B^2}{(1+B)^2}\right)\right]}$$

Where:

$$DA_{tce-event}\left(\frac{\mu g}{cm^2 \cdot event}\right)$$

$$= \frac{TR \times AT_{resw}\left(\frac{365\ days}{year} \times LT(70\ years)\right) \times \left(\frac{1000 \mu g}{mg}\right)}{\left(\frac{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1}}{GIABS}\right) \times \left[\left(CAF_0(0.804) \times DFW_{resw-adj}\left(2721670\,\frac{events \cdot cm^2}{kg}\right)\right) + \left(MAF_0(0.202) \times DFWM_{res-adj}\left(8419740\,\frac{events \cdot cm^2}{kg}\right)\right)\right]}$$

Where:

$$DFW_{res-adj}\left(2721670\,\frac{cm^2 \cdot event}{kg}\right)$$

$$= \frac{EV_{reswc}\left(\frac{1\ events}{day}\right) \times ED_{reswc}(6\ years) \times EF_{reswc}\left(350\,\frac{days}{year}\right) \times SA_{reswc}(6{,}378\ cm^2)}{BW_{reswc}(15\ kg)}$$

$$+ \frac{EV_{reswa}\left(\frac{1\ events}{day}\right) \times ED_{reswa}(20\ years) \times EF_{reswa}\left(350\,\frac{days}{year}\right) \times SA_{reswa}(20{,}900\ cm^2)}{BW_{reswa}(80 kg)}$$

And:

$$DFWM_{res-adj}\left(8419740\frac{events\cdot cm^2}{kg}\right)$$
$$=\left[\left(\frac{EV_{0-2}\left(\frac{1\ events}{day}\right)\times ED_{0-2}(2\ years)\times EF_{0-2}\left(350\frac{days}{year}\right)\times SA_{0-2}(6{,}378\ cm^2)\times 10}{BW_{0-2}(15\ kg)}\right)\right.$$
$$+\left(\frac{EV_{2-6}\left(\frac{1\ events}{day}\right)\times ED_{2-6}(4\ years)\times EF_{2-6}\left(350\frac{days}{year}\right)\times SA_{2-6}(6{,}378\ cm^2)\times 3}{BW_{2-6}(15\ kg)}\right)$$
$$+\left(\frac{EV_{6-16}\left(\frac{1\ events}{day}\right)\times ED_{6-16}(10\ years)\times EF_{6-16}\left(350\frac{days}{year}\right)\times SA_{6-16}(20{,}900\ cm^2)\times 3}{BW_{6-16}(80\ kg)}\right)$$
$$\left.+\left(\frac{EV_{16-30}\left(\frac{1\ events}{day}\right)\times ED_{16-26}(10\ years)\times EF_{16-26}\left(350\frac{days}{year}\right)\times SA_{16-26}(20{,}900\ cm^2)\times 1}{BW_{16-26}(80\ kg)}\right)\right]$$

And:

$$ET^{der}_{resw-madj}\left(0.67077\frac{hours}{event}\right)$$
$$=\frac{ET^{der}_{0-2}\left(0.54\frac{hours}{event}\right)\times ED_{0-2}(2\ years)+ET^{der}_{2-6}\left(0.54\frac{hours}{event}\right)\times ED_{2-6}(4\ years)}{+ET^{der}_{6-16}\left(0.71\frac{hours}{event}\right)\times ED_{6-16}(10\ years)+ET^{der}_{16-26}\left(0.71\frac{hours}{event}\right)\times ED_{16-26}(10\ years)}$$
$$ED_{0-2}(2\ years)+ED_{2-6}(4\ years)+ED_{6-16}(10\ years)+ED_{16-26}(10\ years)$$

2.5.3 Inhalation

$$CL_{water-tce-inh}\left(\frac{\mu g}{L}\right)$$
$$=\frac{TR\times AT_{resw}\left(\frac{365\ days}{year}\times \mathrm{LT}(70\ years)\right)}{ET^{inh}_{resw}\left(\frac{24\ hours}{day}\right)\times\frac{1\ day}{24\ hours}\times \mathrm{K}\left(0.5\frac{L}{m^3}\right)\times \mathrm{IUR}\left(\frac{\mu g}{m^3}\right)^{-1}}$$
$$\times\left[\begin{array}{c}\left(EF_{resw}\left(350\frac{days}{year}\right)\times ED_{resw}(26\ years)\times CAF_i(0.756)\right)+\left(ED_{0-2}(2\ years)\times EF_{0-2}\left(350\frac{days}{year}\right)\times MAF_i(0.244)\times 10\right)\\ +\left(ED_{2-6}(4\ years)\times EF_{2-6}\left(350\frac{days}{year}\right)\times MAF_i(0.244)\times 3\right)+\left(ED_{6-16}(10\ years)\times EF_{6-16}\left(350\frac{days}{year}\right)\times MAF_i(0.244)\times 3\right)\\ +\left(ED_{16-26}(10\ years)\times EF_{16-26}\left(350\frac{days}{year}\right)\times MAF_i(0.244)\times 1\right)\end{array}\right]$$

$$CAF_i(0.756)=\frac{IUR\left(3.1\times 10^{-6}\left(\frac{\mu g}{m^3}\right)^{-1}\right)\ NHL+Liver\ Unit\ Risk\ Estimate}{IUR\left(4.1\times 10^{-6}\left(\frac{\mu g}{m^3}\right)^{-1}\right)\ Adult-Based\ Unit\ Risk\ Estimate}$$

$$MAF_i(0.244)=\frac{IUR\left(1\times 10^{-6}\left(\frac{\mu g}{m^3}\right)^{-1}\right)\ Kidney\ Unit\ Risk\ Estimate}{IUR\left(4.1\times 10^{-6}\left(\frac{\mu g}{m^3}\right)^{-1}\right)\ Adult-Based\ Unit\ Risk\ Estimate}$$

2.5.4 Total

$$CL_{water-tce-tot}(\mu g/L) = \frac{1}{\frac{1}{CL_{water-tce-ing}} + \frac{1}{CL_{water-tce-der}} + \frac{1}{CL_{water-tce-inh}}}$$

3.0 Soil Cleanup Level Equations for Residential Soil

3.1 Equations for Non-Carcinogenic Compounds

Cleanup level equations for exposure to non-carcinogenic compounds in soil are presented below. The terms used in the equations are defined in Appendix B. The equations include exposure routes via ingestion, inhalation of particulates, and dermal contact, which are then totaled to produce a final value.

3.1.1 Incidental Ingestion of Soil

$$CL_{soil-nc-ing}(mg/kg) = \frac{THQ \times AT_{ressc}\left(\frac{365\ days}{year} \times ED_{ressc}(6\ years)\right) \times BW_{ressc}(15\ kg)}{EF_{ressc}\left(\frac{days}{year}\right) \times ED_{ressc}(6\ year) \times \frac{\text{RBA}}{RfD_0\left(\frac{mg}{kg \cdot day}\right)} \times IRS_{ressc}\left(200\,\frac{mg}{day}\right) \times \frac{10^{-6}kg}{mg}}$$

3.1.2 Dermal Contact with Soil

$$CL_{soil-nc-der}(mg/kg) = \frac{THQ \times AT_{ressc}\left(\frac{365\ days}{year} \times ED_{ressc}(6\ years)\right) \times BW_{ressc}(15\ kg)}{EF_{ress}\left(\frac{days}{year}\right) \times ED_{ressc}(6\ year) \times \frac{1}{\left(RfD_0\left(\frac{mg}{kg \cdot day}\right) \times GIABS\right)} \times SA_{ressc}\left(2373\,\frac{cm^2}{day}\right) \times AF_{ressc}\left(0.2\,\frac{mg}{cm^2}\right) \times ABS_d \times \frac{10^{-6}kg}{mg}}$$

3.1.3 Inhalation of Particulates Emitted from Soil

$$CL_{soil-nc-inh}(mg/kg) = \frac{THQ \times AT_{ressc}\left(\frac{365\ days}{year} \times ED_{ressc}(6\ years)\right)}{EF_{ressc}\left(\frac{days}{year}\right) \times ED_{ressc}(6\ year) \times ET_{ressc}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times \frac{1}{RfC\left(\frac{mg}{m^3}\right)} \times \left(\frac{1}{VF_s\left(\frac{m^3}{Kg}\right)} + \frac{1}{PEF_w\left(\frac{m^3}{Kg}\right)}\right)}$$

3.1.4 Total Non-carcinogenic Risk for All Soil Exposure Pathways

$$CL_{soil-nc-tot}(mg/kg) = \frac{1}{\frac{1}{CL_{soil-nc-ing}} + \frac{1}{CL_{soil-nc-der}} + \frac{1}{CL_{soil-nc-inh}}}$$

3.2 Equations for Carcinogenic Compounds

Cleanup level equations for exposure to carcinogenic compounds in soil are presented below. The equations include exposure routes via ingestion, inhalation of particulates, and dermal contact, which are then totaled to produce a final value.

3.2.1 Incidental Ingestion of Soil

$$CL_{soil-ca-ing}(mg/kg) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1} \times \text{RBA} \times IFS_{res-adj}\left(28350\frac{mg}{kg}\right) \times \left(\frac{10^{-6}kg}{mg}\right)}$$

Where:

$$IFS_{res-adj}\left(28350\frac{mg}{kg}\right) = \frac{ED_{ressc}(6\ years) \times EF_{ressc}\left(\frac{days}{year}\right) \times IRS_{ressc}\left(\frac{200\ mg}{day}\right)}{BW_{ressc}(15\ kg)} + \frac{[ED_{ress}(26\ years) - ED_{ressc}(6\ years)] \times EF_{ressa}\left(\frac{days}{year}\right) \times IRS_{ressa}\left(\frac{100\ mg}{day}\right)}{BW_{ressa}(80\ kg)}$$

3.2.2 Dermal Contact with Soil

$$CL_{res-sol-ca-der}(mg/kg) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{\left(\frac{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1}}{GIABS}\right) \times DFS_{res-adj}\left(79758\frac{mg}{kg}\right) \times ABS_d \times \left(\frac{10^{-6}kg}{mg}\right)}$$

Where:

$$DFS_{res-adj}\left(79758\frac{mg}{kg}\right) = \frac{ED_{ressc}(6\ years) \times EF_{ressc}\left(\frac{days}{year}\right) \times SA_{ressc}\left(2373\frac{cm^2}{day}\right) \times AF_{ressc}\left(0.2\frac{mg}{cm^2}\right)}{BW_{ressc}(15\ kg)} + \frac{[ED_{ress}(26\ years) - ED_{ressc}(6\ years)] \times EF_{ressa}\left(\frac{days}{year}\right) \times SA_{ressa}\left(6032\frac{cm^2}{day}\right) \times AF_{ressa}\left(0.07\frac{mg}{cm^2}\right)}{BW_{ressa}(80\ kg)}$$

3.2.3 Inhalation of Particulates Emitted from Soil

$$CL_{soil-ca-inh}(mg/kg) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times \left(\frac{1000\ \mu g}{mg}\right) \times EF_{ress}\left(\frac{days}{year}\right) \times \left(\frac{1}{VF_s\left(\frac{m^3}{kg}\right)} + \frac{1}{PEF_w\left(\frac{m^3}{kg}\right)}\right) \times ED_{ress}(26\ year) \times ET_{ress}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right)}$$

3.2.4 Total Carcinogenic Risk for All Soil Exposure Pathways

$$CL_{soil-ca-tot}(mg/kg) = \frac{1}{\frac{1}{CL_{soil-ca-ing}} + \frac{1}{CL_{soil-ca-der}} + \frac{1}{CL_{soil-ca-inh}}}$$

3.3 Equations for Mutagenic Compounds

Cleanup level equations for exposure to mutagenic compounds in soil are presented below. For these compounds, the exposure rates take into account age-specific susceptibility to mutagens through the use of an age dependent adjustment factor (ADAF). The equations include exposure routes via ingestion, inhalation of particulates, and dermal contact, which are then totaled to produce a final value.

3.3.1 Incidental Ingestion of Soil

$$CL_{soil-mu-ing}(mg/kg) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1} \times RBA \times IFSM_{res-adj}\left(128700\frac{mg}{kg}\right) \times \left(\frac{10^{-6}kg}{mg}\right)}$$

Where:

$$IFSM_{res-adj}\left(128700\frac{mg}{kg}\right) = \frac{ED_{0-2}(2\ years) \times EF_{0-2}\left(\frac{days}{year}\right) \times IRS_{0-2}\left(200\frac{mg}{day}\right) \times 10}{BW_{0-2}(15\ kg)} + \frac{ED_{2-6}(4\ years) \times EF_{2-6}\left(\frac{days}{year}\right) \times IRS_{2-6}\left(200\frac{mg}{day}\right) \times 3}{BW_{2-6}(15\ kg)} + \frac{ED_{6-16}(10\ years) \times EF_{6-16}\left(\frac{days}{year}\right) \times IRS_{6-16}\left(100\frac{mg}{day}\right) \times 3}{BW_{6-16}(80\ kg)} + \frac{ED_{16-26}(10\ years) \times EF_{16-26}\left(\frac{days}{year}\right) \times IRS_{16-26}\left(100\frac{mg}{day}\right) \times 1}{BW_{16-26}(80\ kg)}$$

3.3.2 Dermal Contact with Soil

$$CL_{soil-mu-der}(mg/kg) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{\left(\frac{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1}}{GIABS}\right) \times DFSM_{res-adj}\left(330372\frac{mg}{kg}\right) \times ABS_d \times \left(\frac{10^{-6}kg}{mg}\right)}$$

Where:

$$DFSM_{res-adj}\left(330372\frac{mg}{kg}\right) = \frac{ED_{0-2}(2\ years) \times EF_{0-2}\left(\frac{days}{year}\right) \times AF_{0-2}\left(0.2\frac{mg}{cm^2}\right) \times SA_{0-2}\left(2373\frac{cm^2}{day}\right) \times 10}{BW_{0-2}(15\ kg)} + \frac{ED_{2-6}(4\ years) \times EF_{2-6}\left(\frac{days}{year}\right) \times AF_{2-6}\left(0.2\frac{mg}{cm^2}\right) \times SA_{2-6}\left(2373\frac{cm^2}{day}\right) \times 3}{BW_{2-6}(15\ kg)} + \frac{ED_{6-16}(10\ years) \times EF_{6-16}\left(\frac{days}{year}\right) \times AF_{6-16}\left(0.07\frac{mg}{cm^2}\right) \times SA_{6-16}\left(6032\frac{cm^2}{day}\right) \times 3}{BW_{6-16}(80\ kg)} + \frac{ED_{16-26}(10\ years) \times EF_{16-26}\left(\frac{days}{year}\right) \times AF_{16-26}\left(0.07\frac{mg}{cm^2}\right) \times SA_{16-26}\left(6032\frac{cm^2}{day}\right) \times 1}{BW_{16-26}(80\ kg)}$$

3.3.3 Inhalation of Particulates Emitted from Soil

$$CL_{soil-mu-inh}(mg/kg) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times \left(\frac{1}{VF_s\left(\frac{m^3}{kg}\right)} + \frac{1}{PEF_w\left(\frac{m^3}{kg}\right)}\right) \times \left(\frac{1000\ \mu g}{mg}\right) \times \left(\begin{array}{l}\left(ED_{0-2}(2\ years) \times EF_{0-2}\left(\frac{days}{year}\right) \times ET_{0-2}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times 10\right) + \left(ED_{2-6}(4\ years) \times EF_{2-6}\left(\frac{days}{year}\right) \times ET_{2-6}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times 3\right) + \\ \left(ED_{6-16}(10\ years) \times EF_{6-16}\left(\frac{days}{year}\right) \times ET_{6-16}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times 3\right) + \left(ED_{16-26}(10\ years) \times EF_{16-26}\left(\frac{days}{year}\right) \times ET_{6-16}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times 1\right)\end{array}\right)}$$

3.3.4 Total Mutagenic Risk for All Soil Exposure Pathways

$$CL_{soil-mu-tot}(mg/kg) = \frac{1}{\frac{1}{CL_{soil-mu-ing}} + \frac{1}{CL_{soil-mu-der}} + \frac{1}{CL_{soil-mu-inh}}}$$

3.4 Equations for Vinyl Chloride

Cleanup level equations for exposure to vinyl chloride in soil are presented below. The equations include exposure routes via ingestion, inhalation of particulates, and dermal contact, which are then totaled to produce a final value.

3.4.1 Incidental Ingestion of Soil

$$CL_{soil-vc-ing}\left(\frac{mg}{kg}\right) = \frac{TR}{\left(\frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1} \times \text{RBA} \times IFS_{res-adj}\left(28350\frac{mg}{kg}\right) \times \frac{10^{-6}kg}{mg}}{AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}\right) + \left(\frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1} \times \text{RBA} \times IRS_{ressc}\left(200\frac{mg}{day}\right) \times \frac{10^{-6}kg}{mg}}{BW_{ressc}(15\ kg)}\right)}$$

Where $IFS_{res\text{-}adj}$ = $IFS_{res\text{-}adj}$ from Section 3.2.1

3.4.2 Dermal Contact with Soil

$$CL_{soil-vc-der}\left(\frac{mg}{kg}\right) = \frac{TR}{\left(\frac{\frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1}}{GIABS} \times DFS_{res-adj}\left(79758\frac{mg}{kg}\right) \times ABS_d \times \frac{10^{-6}kg}{mg}}{AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}\right) + \left(\frac{\frac{CSF_0\left(\frac{mg}{kg\cdot day}\right)^{-1}}{GIABS} \times SA_{ressc}\left(2373\frac{cm^2}{day}\right) \times AF_{ressc}\left(0.2\frac{mg}{cm^2}\right) \times ABS \times \frac{10^{-6}kg}{mg}}{BW_{ressc}(15\ kg)}\right)}$$

Where $DFS_{res\text{-}adj}$ = $DFS_{res\text{-}adj}$ from 3.2.2

3.4.3 Inhalation of Particulates Emitted from Soil

$$CL_{soil-vc-inh}\left(\frac{mg}{kg}\right) = \frac{TR}{\left(\frac{IUR\left(\frac{\mu g}{m^3}\right)^{-1} \times EF_{ress}\left(\frac{days}{year}\right) \times ED_{ress}(26\ years) \times ET_{ress}\left(\frac{24\ hours}{day}\right) \times \left(\frac{1\ day}{24\ hours}\right) \times \left(\frac{1000\ \mu g}{mg}\right)}{AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right) \times VF_s\left(\frac{m^3}{kg}\right)}\right) + \left(\frac{IUR\left(\frac{\mu g}{m^3}\right)^{-1}}{VF_s\left(\frac{m^3}{kg}\right)} \times \left(\frac{1000\ \mu g}{mg}\right)\right)}$$

3.4.4 Total Vinyl Chloride Risk for All Soil Exposure Pathways

$$CL_{soil-vc-tot}(mg/kg) = \frac{1}{\frac{1}{CL_{soil-vc-ing}} + \frac{1}{CL_{soil-vc-der}} + \frac{1}{CL_{soil-vc-inh}}}$$

3.5 Trichloroethylene

3.5.1 Ingestion

$$CL_{soil-tce-ing}(mg/kg) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1} \times \text{RBA} \times \frac{10^{-6} kg}{mg} \times \left[\begin{array}{l}\left(CAF_O(0.804) \times IFS_{res-adj}\left(28350\frac{mg}{kg}\right)\right) \\ +MAF_O(0.202) \times IFSM_{res-adj}\left(128700\frac{mg}{kg}\right)\end{array}\right]}$$

Where:

CAF_O = CAF_O from Section 2.5.1

MAF_O = MAF_O from Section 2.5.1

$IFS_{res\text{-}adj}$ = $IFS_{res\text{-}adj}$ from Section 3.2.1

$IFSM_{res\text{-}adj}$ = $IFSM_{res\text{-}adj}$ from Section 3.3.1

3.5.2 Dermal

$$CL_{soil-\text{tce}-der}\left(\frac{mg}{kg}\right) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times LT(70\ years)\right)}{\left(\frac{CSF_0\left(\frac{mg}{kg \cdot day}\right)^{-1}}{GIABS}\right) \times \frac{10^{-6} kg}{mg}\left[\begin{array}{l}\left(CAF_O(0.804) \times DFS_{res-adj}\left(79758\frac{mg}{kg}\right) \times ABS_d\right) \\ +\left(MAF_O(0.202) \times DFSM_{res-adj}\left(330372\frac{mg}{kg}\right) \times ABS_d\right)\end{array}\right]}$$

Where:

$DFS_{res\text{-}adj}$ = $DFS_{res\text{-}adj}$ from Section 3.2.2

$DFSM_{res\text{-}adj}$ = $DFSM_{res\text{-}adj}$ from Section 3.3.2

3.5.3 Inhalation

$$CL_{water-tce-inh}\left(\frac{\mu g}{L}\right) = \frac{TR \times AT_{ress}\left(\frac{365\ days}{year} \times \text{LT}(70\ years)\right)}{\text{IUR}\left(\frac{\mu g}{m^3}\right)^{-1} \times \left(\frac{1}{VF_s\left(\frac{m^3}{kg}\right)} + \frac{1}{PEF_w\left(\frac{m^3}{kg}\right)}\right) \times \frac{1000\ \mu g}{mg} \times \frac{day}{24\ hours}}$$

$$\times \left[\begin{array}{c}\left(EF_{ress}\left(\frac{days}{year}\right) \times ED_{ress}(26\ years) \times ET_{ress}\left(\frac{24\ hours}{day}\right) \times CAF_i(0.756)\right) \\ +\left(ED_{0-2}(2\ years) \times EF_{0-2}\left(\frac{days}{year}\right) \times ET_{0-2}\left(\frac{24\ hours}{day}\right) \times MAF_i(0.244) \times 10\right) \\ +\left(ED_{2-6}(4\ years) \times EF_{2-6}\left(\frac{days}{year}\right) \times ET_{2-6}\left(\frac{24\ hours}{day}\right) \times MAF_i(0.244) \times 3\right) \\ +\left(ED_{6-16}(10\ years) \times EF_{6-16}\left(\frac{days}{year}\right) \times ET_{6-16}\left(\frac{24\ hours}{day}\right) \times MAF_i(0.244) \times 3\right) \\ +\left(ED_{16-26}(10\ years) \times EF_{16-26}\left(\frac{days}{year}\right) \times ET_{16-26}\left(\frac{24\ hours}{day}\right) \times MAF_i(0.244) \times 1\right)\end{array}\right]$$

3.5.4 Total

$$CL_{soil-tce-tot}(mg/kg) = \frac{1}{\frac{1}{CL_{soil-tce-ing}} + \frac{1}{CL_{soil-tce-der}} + \frac{1}{CL_{soil-tce-inh}}}$$

4.0 Migration to Groundwater Cleanup Levels

4.1 Soil-Water Partitioning Equation for Migration to Groundwater

The standard default attenuation factor (AF) used to determine the cleanup standards is: AF = 4. The AF may be modified on a chemical-specific basis. The standard dilution factor is DF = 3.3 (see equation below). The standard default dilution attenuation factor (DAF) used to determine the cleanup standards is: DAF (DF x AF) = 13.2. The standard default value for fractional organic carbon (foc) is 0.001 (0.1%). Exhibit C- 4 of the Soil Screening Guidance (U.S. EPA. 1996a) provides pH-specific soil-water partition coefficients (Kd) for metals. Site-specific soil pH measurements can be used to select appropriate Kd values for these metals. Where site-specific soil pH values are not available, values corresponding to a pH of 6.8 should be used. The soil-water partitioning equation is shown below:

$$CL\,(mg/kg) = C_w\left(\frac{mg}{L}\right) \times DAF \times \left[K_d\left(\frac{L}{kg}\right) + \left(\frac{\left(\theta_w\left(\frac{L_{water}}{L_{soil}}\right) + \theta_a\left(\frac{L_{air}}{L_{soil}}\right) \times H'\right)}{P_b\left(\frac{1.5kg}{L}\right)}\right)\right]$$

Where:

$$\theta_a\left(0.13\frac{L_{air}}{L_{soil}}\right) = n\left(0.43\frac{L_{water}}{L_{soil}}\right) - \theta_w\left(0.3\frac{L_{water}}{L_{soil}}\right);$$

$$n\left(0.43\frac{L_{pore}}{L_{soil}}\right) = 1 - \left(\frac{\rho_b\left(\frac{1.5kg}{L}\right)}{\rho_s\left(\frac{2.65kg}{L}\right)}\right) and$$

$$K_d\left(\frac{L}{kg}\right) = K_{oc}\left(\frac{L}{kg}\right) \times f_{oc}(0.001\ g/g)$$

5.0 Explanation of Supporting Equations and Parameters

5.1 Derivation of the Volatilization Factor

The soil-to-air volatilization factor (VF) is used to define the relationship between the concentration of the contaminant in soil and the flux of the volatilized contaminant to air. VF is calculated from the equation below using chemical-specific properties and either site-measured or default values for soil moisture, dry bulk density, and fraction of organic carbon in soil. The Soil Screening Guidance: User's Guide (U.S. EPA. 1996b) describes how to develop site measured values for these parameters.

The VF is only calculated for volatile organic compounds (VOCs). VOCs, for the purpose of this document, generally are chemicals with a Henry's Law constant greater than or equal to 1 x 10^{-5} atm-m^3/mole and a molecular weight of less than 200 g/mol. Exceptions are: Mercury (elemental); Pyrene; Dibromochloromethane; and 1,2-Dibromo-3-chloropropane.

Because of its reliance on Henry's law, the VF model applies only when the contaminant concentration in soil is at or below saturation (i.e., no free-phase contaminant is present). Soil saturation (Csat) corresponds to the contaminant concentration in soil at which the adsorptive limits of the soil particles and the solubility limits of the available soil moisture have been reached. Above this point, pure liquid-phase contaminant is expected in the soil. If the cleanup level calculated using the VF exceeds the calculated Csat value, the cleanup level is set equal to Csat in accordance with the "Soil Screening Guidance" (U.S. EPA 1996a, 1996b). The equation for the soil saturation limit is presented in section 5.4.

Chemical specific default dermal absorption values are provided in Appendix A and obtained from Supplemental Guidance for Dermal Risk Assessment," Part E of Risk Assessment Guidance for Superfund Human Health Evaluation Manual (Volume I), July 2004 (U.S. EPA. 2004). Chemicals without default dermal absorption values and considered VOC are not quantified. The rationale for this is that in the considered soil exposure scenarios, volatile organic compounds would tend to be volatilized from the soil on skin and should be accounted for via inhalation routes in the combined exposure pathway analysis. Further, a chemical must be a VOC in order to be included in the calculation of groundwater inhalation.

$$VF\left(\frac{m^3_{air}}{kg_{soil}}\right) = \frac{\frac{Q}{C_{vol}}\left(\frac{\frac{g}{m^2 \cdot s}}{\frac{kg}{m^3}}\right) \times \left(3.14 \times D_A\left(\frac{cm^2}{s}\right) \times T(s)\right)^{1/2} \times 10^{-4}\left(\frac{m^2}{cm^2}\right)}{2 \times \rho_b\left(\frac{g}{cm^3}\right) \times D_A\left(\frac{cm^2}{s}\right)}$$

Where: $\frac{Q}{C_{vol}}\left(\frac{\frac{g}{m^2 \cdot s}}{\frac{kg}{m^3}}\right) = A \times exp\left[\frac{(lnA_S(acre)-B)^2}{C}\right]$

And:

$$D_A\left(\frac{cm^2}{s}\right)=\frac{\left[\frac{\left(\theta_a\left(\frac{L_{air}}{L_{soil}}\right)^{\frac{10}{3}}\times D_{ia}\left(\frac{cm^2}{s}\right)\times H'+\theta_w\left(0.15\frac{L_{water}}{L_{soil}}\right)^{\frac{10}{3}}\times D_{iw}\left(\frac{cm^2}{s}\right)\right)}{n^2\left(\frac{L_{pore}}{L_{soil}}\right)}\right]}{\rho_b\left(1.5\frac{g}{cm^3}\right)\times K_d\left(\frac{cm^3}{g}\right)+\theta_w\left(0.15\frac{L_{water}}{L_{soil}}\right)+\theta_a\left(\frac{L_{air}}{L_{soil}}\right)\times H'}$$

5.2 Selection of Compounds for Dermal Absorption

The single soil cleanup level for each climate zone accounts for the inhalation, ingestion and dermal contact pathways. For those contaminants that are unlikely to undergo significant dermal absorption, the final cleanup level will only reflect the soil ingestion and inhalation pathways.

Dermal absorption of contaminants in soil is calculated based on the Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment (EPA, 2004). Where specific absorption factors were not available for an organic compound and it is not considered a volatile, an absorption fraction of 0.10 is applied. It is generally accepted that volatile compounds evaporate from skin before significant absorption occurs and are addressed through the inhalation exposure pathway.

5.3 Particulate Emission Factor (PEF)

Inhalation of contaminants adsorbed to respirable particles (PM10) was assessed using a default PEF equal to 1.36 x 10^9 m^3/kg. This equation relates the contaminant concentration in soil with the concentration of respirable particles in the air due to fugitive dust emissions from contaminated soils. The generic PEF was derived using default values that correspond to a receptor point concentration of approximately 0.76 µg/m^3. The relationship is derived by Cowherd et al (1985) for a rapid assessment procedure applicable to a typical hazardous waste site, where the surface contamination provides a relatively continuous and constant potential for emission over an extended period of time (e.g., years). This represents an annual average emission rate based on wind erosion that should be compared with chronic health criteria; it is not appropriate for evaluating the potential for more acute exposures. Definitions of the input variables are in the Standard Defaults Table 7 in Appendix B.

With the exception of specific heavy metals, the PEF does not appear to significantly affect most soil cleanup levels. The equation forms the basis for deriving a generic PEF for the inhalation pathway. For more details regarding specific parameters used in the PEF model, refer to Soil Screening Guidance: Technical Background Document (U.S. EPA. 1996a). The use of alternate values on a specific site should be justified and presented in an Administrative Record if considered in Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) remedy selection.

Note: the generic PEF evaluates wind-borne emissions and does not consider dust emissions from traffic or other forms of mechanical disturbance that could lead to greater emissions than assumed here.

$$PEF_w\left(\frac{m^3_{air}}{kg_{soil}}\right) = \frac{Q}{\mathrm{C_w}}\left(\frac{\frac{g}{m^2 \cdot s}}{\frac{kg}{m^3}}\right) \times \frac{3{,}600\,\frac{s}{hour}}{0.036 \times (1 - \mathrm{V}) \times \left(\frac{\mathrm{U_m}\left(\frac{m}{s}\right)}{\mathrm{U_t}\left(\frac{m}{s}\right)}\right)^3 \times F(X)}$$

Where:

$$\frac{Q}{C_w} = A \times exp\left[\frac{(lnA_S(acre) - B)^2}{C}\right]$$

5.4 Derivation of the Soil Saturation Limit (C_{sat})

The soil saturation concentration, Csat, corresponds to the contaminant concentration in soil at which the absorptive limits of the soil particles, the solubility limits of the soil pore water, and saturation of soil pore air have been reached. Above this concentration, the soil contaminant may be present in free phase (i.e., nonaqueous phase liquids (NAPLs) for contaminants that are liquid at ambient soil temperatures and pure solid phases for compounds that are solid at ambient soil temperatures). Csat is not calculated for chemicals that are solid at ambient soil temperatures. The following decision criteria was established from the Soil Screening Guidance User's Guide, Table C-3: if melting point is less than 20 °C, chemical is a liquid; if melting point is above 20 °C, chemical is solid (U.S. EPA. 1996b).

The equation below is used to calculate C_{sat}; for each volatile contaminant. As an update to RAGS HHEM, Part B (U.S. EPA. 1991a), this equation takes into account the amount of contaminant that is in the vapor phase in soil in addition to the amount dissolved in the soil's pore water and sorbed to soil particles.

Chemical-specific C_{sat} concentrations must be compared with each VF-based cleanup level (CL) because a basic principle of the volatilization model is not applicable when free-phase contaminants are present. How these cases are handled depends on whether the contaminant is liquid or solid at ambient temperatures. Liquid contaminants that have a VF-based CL that exceeds the C_{sat} concentration are set equal to $C_{sat;}$ whereas for solids (e.g., PAHs), soil cleanup decisions are based on the appropriate CLs for other pathways of concern at the site (e.g., ingestion).

$$C_{sat} = \frac{S\left(\frac{mg}{L}\right)}{\rho_b\left(\frac{kg}{L}\right)} \times \left(K_d\left(\frac{L}{kg}\right) \times \rho_b\left(\frac{kg}{L}\right) + \theta_w\left(\frac{L_{water}}{L_{soil}}\right) + H' \times \theta_a\left(\frac{L_{air}}{L_{soil}}\right)\right)$$

Where:

$$K_d = K_{oc}\left(\frac{L}{kg}\right) \times f_{oc}\left(0.001\frac{g}{g}\right)$$

$$\theta_a\left(\frac{L_{air}}{L_{soil}}\right) = n\left(\frac{L_{pore}}{L_{soil}}\right) - \theta_w\left(\frac{L_{water}}{L_{soil}}\right) \; and \; n = 1 - \left(\frac{\rho_b\left(\frac{kg}{L}\right)}{\rho_s\left(\frac{kg}{L}\right)}\right)$$

5.5 Derivation of Dilution Factor

The DEC sets a default dilution factor of 3.3 generated by the following equation:

$$Dilution\ Factor\ (DF) = 1 + \frac{K\left(876\frac{m}{year}\right) \times i\left(0.002\frac{m}{m}\right) \times d(5.5m)}{I\left(0.13\frac{m}{year}\right) \times L(32m)}$$

Where *d*, the mixing zone, is calculated as follows:

$$d(m) = (0.0112 \times L(32m)^2)^{0.5} + d_a(10m) \times \left[1 - exp\left(\frac{-L(32m) \times I\left(0.13\frac{m}{year}\right)}{K\left(876\frac{m}{year}\right) \times i\left(0.002\frac{m}{m}\right) \times d_a(10m)}\right)\right]$$

5.6 Groundwater

5.6.1 B

B is the dimensionless ratio of the permeability coefficient of a compound through the stratum corneum relative to its permeability coefficient across the viable epidermis.

$$B(unitless) = \frac{K_P\left(\frac{cm}{hour}\right)\sqrt{MW\left(\frac{g}{mol}\right)}}{2.6}$$

5.6.2 τ_{event}

τevent is the lag time per event

$$\tau_{event}\left(\frac{hours}{event}\right) = \frac{1}{6 \times 10^{(0.2\ -\ 0.0056 \times MW)}}$$

5.6.3 t*

t* is the time to reach steady state.

$$IF\ B \leq 0.6, then\ t^*(hours) = 2.4 \times \tau_{event}\left(\frac{hours}{event}\right)$$

$$IF\ B > 0.6, then\ t^*(hours) = 6 \times \tau_{event}\left(\frac{hours}{event}\right) \times \left(b - \sqrt{b^2 - c^2}\right)$$

Where

$$b = \frac{2 \times (1 + B)^2}{\pi} - c$$

And $c = \frac{1+3B+3B^2}{3(1+B)}$

6.0 Petroleum Fraction Equations

Cleanup levels for the petroleum fractions presented for soil in Table B2 of 18 AAC 75.340, and for groundwater in Table C of 18 AAC 75.345, are calculated using the following set of equations. These equations were developed using the 1996 EPA Soil Screening Guidance, and remain unchanged from the last update of these cleanup level calculation procedures in June of 2008. Therefore, they do not incorporate the exposure parameters, toxicity values and assumptions of the RSL equations for non-petroleum compounds that are presented in the preceding sections of these procedures. DEC expects to update the equations for calculating the petroleum cleanup criteria as part of a future regulatory update. For chemical specific parameters for the petroleum fractions, refer to Table 1 in Section 6.9.

6.1 Groundwater Cleanup Levels for Petroleum Contaminants

Previously referred to as **Equation 15.**

Cleanup Level (mg/L) = $\frac{THQ \times RfD_o \times BW \times AT \times 365\ d/yr}{IR \times EF \times ED \times A}$	
Parameter/Definition (units)	Default
THQ/target hazard quotient (unitless)	1
BW/body weight (kg)	70
AT/averaging time (yr)	30
RfD_o/oral reference dose (mg/kg-d)	Chemical-specific (See Table 1)
EF/exposure frequency (d/yr)	350
ED/exposure duration (yr)	30
IR/ ingestion rate (L/d)	2
A/absorption factor	1
For non-carcinogens, averaging time is equal to exposure duration.	

6.2 Residential Soil Cleanup Levels for Ingestion of Petroleum Fractions

Previously referred to as **Equation 16**.

Cleanup Level (mg/kg) = $\frac{\text{THQ x BW x AT x 365 d/yr}}{1/\text{RfD}_o \text{x} 10^{-6} \text{ kg/mg x EF x ED x IR}}$

Parameter/Definition (units)	Default
THQ/target hazard quotient (unitless)	1
BW/body weight (kg)	15
AT/averaging time (yr)	6[a]
RfD_o/oral reference dose (mg/kg-d)	Chemical-specific (See Table 1)
EF/exposure frequency (d/yr)	Arctic Zone = 200 d/yr Under 40 Inch Zone = 270 d/yr Over 40 Inch Zone = 330 d/yr
ED/exposure duration (yr)	6
IR/soil ingestion rate (mg/d)	200

[a] For non-carcinogens, averaging time is equal to exposure duration. Cleanup levels are calculated for 6-year childhood exposure.

6.3 Residential Soil Cleanup Levels for Direct Inhalation of Petroleum Fractions

Previously referred to as **Equation 17.**

Cleanup Level (mg/kg) = $\frac{\text{THQ x AT x 365 d/yr}}{\text{EF x ED x [(1/RfC) x (1/VF)]}}$

Parameter/Definition (units)	Default
THQ/target hazard quotient (unitless)	1
AT/averaging time (yr)	30
EF/exposure frequency (d/yr)	Arctic Zone = 200 d/yr Under 40 Inch Zone = 270 d/yr Over 40 Inch Zone = 330 d/yr
ED/exposure duration (yr)	30
RfC/inhalation reference concentration (mg/m^3)	Chemical-specific (See Table 1)
VF/soil-to-air volatilization factor (m^3/kg)	Chemical-specific (See Equation 18)

6.4 Derivation of the Volatilization Factor

Previously referred to as **Equation 18.**

$$VF\ (m^3/kg) = \frac{Q/C \times (3.14 \times D_A \times T)^{1/2} \times 10^4 m^2/cm^2}{(2 \times \rho_b \times D_A)}$$

where

$$D_A = \frac{[(\theta_a^{10/3} D_i H' + \theta_w^{10/3} D_w)/n^2]}{\rho_b K_d + \theta_w + \theta_a H'}$$

Parameter/Definition (units)	Default	
VF/volatilization factor (m^3/kg)	---	
Q/C/inverse of the mean conc. at the center of a 0.5 acre square source (g/m^2-s per kg/m^3)	Arctic Zone	=101.5958
	Under 40 Inch Zone	=90.80
	Over 40 Inch Zone	=82.72
T/exposure interval (s)	8.2×10^8	
ρ_b/dry soil bulk density (g/cm^3)	1.5	
ρ_s/soil particle density (g/cm^3)	2.65	
n/total soil porosity (L_{pore}/L_{soil})	0.43 or 1 - (ρ_b/ρ_s)	
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.15 or $w\rho_b$	
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.28 or n - $w\rho_b$	
D_i/diffusivity in air (cm^2/s)	Chemical-specific (See Table 1)	
H'/ dimensionless Henry's law constant	Chemical-specific (See Table 1)	
w/average soil moisture content $kg_{water}/kg_{soil\text{-}dry}$	0.1 (10%)	
D_w/diffusivity in water (cm^2/s)	Chemical-specific (See Table 1)	
K_d/soil-water partition coefficient (cm^3/g)	K_{oc} x f_{oc} (organics)	
K_{oc}/organic carbon partition coefficient (cm^3/g)	Chemical-specific (See Table 1)	
f_{oc}/organic carbon content of soil (g/g)	0.001 (0.1%)	

6.5 Derivation of the Soil Saturation Limit

Previously referred to as **Equation 19.** Note: The Soil Saturation Limit will be used as an upper limit for petroleum for the Inhalation Pathway Calculations

$$C_{sat}\ (mg/kg) = \frac{S}{\rho_b}\ (K_d\ \rho_b + \theta_w + H'\theta_a)$$

Parameter/Definition (units)	Default
C_{sat}/soil saturation concentration (mg/kg)	---
S/solubility in water (mg/L-water)	Chemical-specific (See Table 1)
ρ_b/dry soil bulk density (kg/L)	1.5
ρ_s/soil particle density (kg/L)	2.65
n/total soil porosity (L_{pore}/L_{soil})	0.434 or 1 - (ρ_b / ρ_s)
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.15 or wρ_b
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.284 or n - wρ_b
K_d/soil-water partition coefficient (L/kg)	K_{oc} x f_{oc}
K_{oc}/soil organic carbon/water partition coefficient (L/kg)	Chemical-specific (See Table 1)
f_{oc}/fraction organic carbon of soil (g/g)	0.001 (0.1%)
w/average soil moisture content $kg_{water}/kg_{soil\text{-}dry}$	0.1 (10%)
H'/Henry's law constant (unitless)	Chemical-specific (See Table 1)

6.6 Soil-Water Partitioning Equation for Migration to Groundwater for Petroleum Fractions

Previously referred to as **Equation 20.**

$$\text{Soil cleanup level (mg/kg)} = C_w\ \{(K_{oc}\ f_{oc}) + (\ (\theta_w + \theta_a H')/\ \rho_b\ )\}$$

Parameter/Definition (units)	Default
C_w/target soil leachate concentration (mg/L)	Groundwater Cleanup Level x (10 + DF), 10 is attenuation factor
K_{oc}/soil organic carbon/water partition coefficient (L/kg)	Chemical-specific (See Table 1)
f_{oc}/fraction organic carbon in soil (g/g)	0.001 (0.1%)
ρ_b/dry soil bulk density (kg/L)	1.5
ρ_s/soil particle density (kg/L)	2.65
n/total soil porosity (L_{pore}/L_{soil})	0.434 or (1 - ρ_b/ρ_s)
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.3 (30%) or wρ_b
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.13 or n -wρ_b
w/average soil moisture content $kg_{water}/kg_{soil\text{-}dry}$	0.2 (20%)
H'/Henry's law constant (unitless)	Chemical Specific (See Table 1)

6.7 Derivation of Dilution Factor

Previously referred to as **Equation 21.**

$DF = 1 + (Kid / IL)$	
Parameter/Definition (units)	Default
DF/dilution factor (unitless)	---
K/aquifer hydraulic conductivity (m/yr)	876 m/yr
i/hydraulic gradient (m/m)	0.002 m/m
d/mixing zone depth (m)	(See Equation 22 below)
I/infiltration rate (m/yr) (calculated as 1/5 * (mean plus one standard deviation of yearly rainfall))	Over 40 Inch Zone =0.6 m/yr Under 40 Inch Zone =0.13 m/yr
L/source length parallel to groundwater flow (m)	32 m
The standard default dilution factors used to determine the cleanup standards are DF = 1.9 for the Over 40 Inch Zone; and DF = 3.3 for the Under 40 Inch Zone.	

6.8 Estimation of Mixing Zone Depth

Previously referred to as **Equation 22**.

$d = (0.0112L^2)^{0.5} + d_a\{1 - \exp[(-LI)/(Kid_a)]\}$	
Parameter/Definition (units)	Default
d/mixing zone depth (m)	---
L/source length parallel to groundwater flow (m)	32 m
I/infiltration rate (m/yr) (calculated as 1/5 * (mean plus one standard deviation of yearly rainfall))	Over 40 Inch Zone =0.6 m/yr Under 40 Inch Zone =0.13 m/yr
K/aquifer hydraulic conductivity (m/yr)	876 m/yr
i/hydraulic gradient (m/m)	0.002
d_a/aquifer thickness (m)	10 m
The standard default mixing zone depths used to determine the cleanup standards are: d = 10.0 for the Over 40 Inch Zone; and d = 5.5 for the Under 40 Inch Zone.	

6.9 Chemical Specific Parameters

Table 1- Chemical Specific Parameters for Petroleum Hydrocarbon Fractions							
HENRY'S LAW CONSTANT, H' (unitless)							
aromatics				$\log_{10}$ H = [-0.23][EC] + 1.7			
aliphatics				$\log_{10}$ H = [0.02][EC] + 1.6			
ORGANIC CARBON PARTITION COEFFICIENT, Koc (ml/g)							
aromatics				$\log_{10}$ Koc = [0.10][EC] + 2.3			
Aliphatics				$\log_{10}$ Koc = [0.45][EC] + 0.43			
Hydrocarbon Range	Equivalent Carbon Number (EC)	Oral Reference Dose (mg/kg/day)	Reference Concentration (mg/m^3)	H' (unitless)	Koc	Diffusivity in Air	Diffusivity in Water
C_6-C_{10} Aliphatics	8	5	18.4	5.75 E+1	1.07 E+4	1 E-1	1 E-5
C_6-C_{10} Aromatics	8	0.2	0.4	7.24 E-1	1.26 E+3	1 E-1	1 E-5
C_{10}-C_{25} Aliphatics	14	0.1	1	7.59 E+1	5.37 E+6	1 E-1	1 E-5
C_{10}-C_{25} Aromatics	14	0.04	0.2	3.02 E-2	5.01 E+3	1 E-1	1 E-5
C_{25}-C_{36} Aliphatics	30.5	2	n/a				
C_{25}-C_{36} Aromatics	30.5	0.03	n/a	4.86 E-6	2.24 E+5	1 E-1	1 E-5

*Note that no values are recommended for the C_{25}-C_{36} aliphatic fraction, as these compounds are essentially immobile in the environment.

6.10 Total Gasoline, Diesel, and Residual Range Organics (GRO, DRO, and RRO) Versus Aromatic/Aliphatic Fractions

Table B2 soil cleanup levels for petroleum hydrocarbons (GRO, DRO, and RRO) are based on Methods AK 101, 102, and 103. The Table B2 GRO, DRO, and RRO levels were derived based on assumed default percentages of aromatic and aliphatic fractions within each carbon range. The Table B2 aliphatic/aromatic fractional cleanup levels were transformed into the GRO, DRO, and RRO levels by dividing the aromatic or aliphatic cleanup level by a corresponding aromatic or aliphatic default percentage.

DEC selected the default compositions of GRO, DRO, and RRO shown in Table 2.

Table 2: Petroleum Hydrocarbon Default Compositions

CARBON RANGE	PERCENT ALIPHATIC*	PERCENT AROMATIC*
GRO - C_6 - C_{10}	70	50
DRO - C_{10} - C_{25}	80	40
RRO - C_{25} - C_{36}	90	30

*Note - Because fuel constituents vary considerably, the default composition of the percent aliphatic and percent aromatics was set at 120% of the total.

For example, the C10-C25 DRO cleanup levels in Table B2 were calculated by dividing the corresponding C10-C25 aliphatic level by 0.80 and also dividing the corresponding C10-C25 aromatic level by 0.40. The lowest result of these two calculations became the method two C10-C25 DRO cleanup level (TPHCWG, 1997).

7.0 Calculating Cleanup Levels under Method Three

Table B1 Contaminants

Alternative residential soil cleanup levels may be developed under method three (18 AAC 75.340(e)) utilizing site-specific data for the soil migration to groundwater pathway. Site-specific parameters that may be modified for Table B1 compounds are listed in Table 3. Equations for the Table B1 contaminants are found in Sections 2.0 through 4.0.

Table 3 – Site-Specific Parameters for Table B1 Compounds

Parameters[1]	Definition (units)	Default Value
f_{oc}	Fractional organic carbon (g/g)	0.001 (1%)
ρ_b	dry soil bulk density (kg/L)	1.5
θw	water-filled soil porosity (L_{water}/L_{soil})	0.15
ρ_s	Soil particle density (kg/L)	2.65
K	Aquifer hydraulic conductivity (m/year)	876
L	Source length parallel to ground water flow (m)	32
d_a	Aquifer thickness (m)	10
I	Hydraulic gradient (m/m)	0.002
I	Infiltration rate (m/yr)	0.13
AF	Attenuation Factor (unitless)	4

Table B2 Petroleum Fractions

Alternative residential soil cleanup levels may be developed under method three (18 AAC 75.340(e)) utilizing site-specific data for the soil migration to groundwater pathway. Site-specific parameters that may be modified for Table B2 petroleum fractions are listed in Table 4. Equations for the petroleum fractions are in Section 6.0.

Table 4 – Site-Specific Parameters for Petroleum Fraction Equations

Parameters[1]	Definition (units)	Default Value
f_{oc}	Fractional organic carbon (g/g)	0.001 (1%)
ρ_b	dry soil bulk density (kg/L)	1.5
n	total soil porosity (L_{pore}/L_{soil})	0.434 or $(1 - \rho_b/\rho_s)$
θw	water-filled soil porosity (L_{water}/L_{soil})	0.15 or $w\rho_b$
θa	air-filled soil porosity (L_{air}/L_{soil})	0.284 or $n - w\rho_b$
w	average soil moisture content kg_{water}/kg_{soil}-dry	0.1 (10%)
K	Aquifer hydraulic conductivity (m/yr)	876 m/yr
i	Hydraulic gradient (m/m)	0.002 m/m
d	Mixing zone depth (m)	See Mixing Zone Depth Equation 22
I	Infiltration rate (m/yr)	>40 inch zone =0.6m/yr <40 inch zone = 0.13 m/yr
L	Source length parallel to groundwater flow (m)	32 m
d_a	Aquifer thickness (m)	10 m

For either Table B1 or B2 contaminants, if a site-specific dry soil bulk density will be used, then the total porosity, air-filled porosity, and water-filled porosity must be calculated using the appropriate equation the respective contaminant. Note that the air-filled soil porosity is the portion of the total porosity of soil containing air. This value is calculated by subtracting the water-filled porosity from the total soil porosity. If a site-specific total soil porosity or water-filled soil porosity is determined for a site, then the air-filled soil porosity should be reviewed to ensure that the sum of the air-filled and water-filled soil porosities equals the total soil porosity.

A standard default mixing zone depth has been adopted by the department for application to Table B1 contaminants. This value cannot be modified. However, for Table B2 petroleum fractions, this value can be modified using site-specific information (see Table 4).

Commercial/Industrial Land Use Scenario

Alternative soil cleanup levels may also be proposed for commercial/industrial exposure scenarios under method three. However, sites where a commercial/industrial exposure scenario is proposed requires an institutional control to ensure that the land use remains commercial industrial in perpetuity, unless a future cleanup action is performed that brings the site into compliance with a residential exposure scenario. Values for parameters that are applied for this scenario are shown in Table 5.

Table 5- Commercial/Industrial Exposure Parameters

Parameters	Definition (units)	Value
AT	averaging time for carcinogens (years)	70 (unchanged from residential)
AT	averaging time for non-carcinogens (years)	25
BW	body weight (kg)	80
ED	exposure duration (years)	25
EF	exposure frequency (days/years)	250 (under 40 inch and over 40 inch zones) 200 (arctic zone)
IRsoil	soil ingestion rate (mg/day)	100 (outdoor worker) 50 (indoor worker)
SA	Surface Area	3527 cm^2
AF	Adherence Factors	0.12 mg/cm^2

For additional guidance on the equations for and calculation of commercial/industrial cleanup levels, reference the EPA Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (U.S. EPA. 2002).

8.0 References

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Appendix A – Toxicity and Chemical Specific Parameters for Non-Petroleum Organic and Inorganic Contaminants

Symbol	Definition
GIABS	Fraction of contaminant absorbed in gastrointestinal tract (unitless) Note: if the GIABS is >50% then it is set to 100% for the calculation of dermal toxicity values.
ABS	Fraction of contaminant absorbed dermally from soil (unitless)
RBA	Relative bioavailability factor
Ingestion SF	Chronic Oral Slope Factor (mg/kg-day)-1
IUR	Chronic Inhalation Unit Risk (µg/m3)-1
RfD	Chronic Oral Reference Dose (mg/kg-day)
RfC	Chronic Inhalation Reference Concentration (mg/m3)
D_{ia}	Diffusivity in air (cm2/hour)
D_{iw}	Diffusivity in water (cm2/hour)
S	Water Solubility Limit (mg/L)
K_d	Soil-water partition coefficient (L/kg) (Koc*foc)
K_{oc}	Soil organic carbon/water partition coefficient (L/kg)
H'	Dimensionless Henry's Law Constant (unitless)
MW	Molecular Weight (g/mol)
FA	Systemically available fraction
K_p	Dermal permeability coefficient in water (cm/hour)
MP	Melting Point (ºC)

Table 6 Chemical Toxicity Parameters

CAS Number[1]	Compound	GIABS	ABS	RBA	Ingestion SF (mg/kg day)$^{-1}$	Ref[2]	Inhalation Unit Risk (µg/m^3)$^{-1}$	Ref[2]	Chronic RfD (mg/kg day)	Ref[2]	Chronic RfC (mg/m^3)	Ref[2]
83-32-9	Acenaphthene	1	0.13	1	-		-		0.06	I	-	
208-96-8	Acenaphthylene[4]	1	0.13	1	-		-		0.03	S	-	
67-64-1	Acetone	1	-	1	-		-		0.9	I	30.880981595092	A
309-00-2	Aldrin	1	-	1	17	I	0.0049	I	0.00003	I	-	
7790-98-9	Ammonium Perchlorate	1	-	1	-		-		0.0007	I	-	
120-12-7	Anthracene	1	0.13	1	-		-		0.3	I	-	
7440-36-0	Antimony (metallic)	0.15	-	1	-		-		0.0004	I	-	
7440-38-2	Arsenic, Inorganic	1	0.03	0.6	1.5	I	0.0043	I	0.0003	I	0.000015	C
7440-39-3	Barium	0.07	-	1	-		-		0.2	I	0.0005	H
56-55-3	Benz[a]anthracene[3]	1	0.13	1	0.73	S	0.00011	C	-		-	
100-52-7	Benzaldehyde	1	-	1	0.004	P	-		0.1	I	-	
71-43-2	Benzene	1	-	1	0.055	I	7.8 x 10^{-6}	I	0.004	I	0.03	I
50-32-8	Benzo[a]pyrene	1	0.13	1	7.3	I	0.0011	C	-		-	
205-99-2	Benzo[b]fluoranthene[3]	1	0.13	1	0.73	S	0.00011	C	-		-	
191-24-2	Benzo[g,h,i]perylene[4]	1	0.13	1	-		-		0.03	S	-	
207-08-9	Benzo[k]fluoranthene[3]	1	0.13	1	0.073	S	0.00011	C	-		-	
65-85-0	Benzoic Acid	1	0.1	1	-		-		4	I	-	
100-51-6	Benzyl Alcohol	1	0.1	1	-		-		0.1	P	-	
7440-41-7	Beryllium and compounds	0.007	-	1	-		0.0024	I	0.002	I	0.00002	I
111-44-4	Bis(2-chloroethyl)ether	1	-	1	1.1	I	0.00033	I	-		-	
117-81-7	Bis(2-ethylhexyl)phthalate	1	0.1	1	0.014	I	2.4 x 10^{-6}	C	0.02	I	-	
108-86-1	Bromobenzene	1	-	1	-		-		0.008	I	0.06	I
75-27-4	Bromodichloromethane	1	-	1	0.062	I	0.000037	C	0.02	I	-	
75-25-2	Bromoform	1	-	1	0.0079	I	1.1 x 10^{-6}	I	0.02	I	-	
74-83-9	Bromomethane	1	-	1	-		-		0.0014	I	0.005	I
106-99-0	Butadiene, 1,3-	1	-	1	3.4	C	0.00003	I	-		0.002	I
71-36-3	Butanol, N-	1	-	1	-		-		0.1	I	-	
85-68-7	Butyl Benzyl Phthalate	1	0.1	1	0.0019	P	-		0.2	I	-	
104-51-8	Butylbenzene, n-	1	-	1	-		-		0.05	P	-	
135-98-8	Butylbenzene, sec-	1	-	1	-		-		0.1	X	-	
98-06-6	Butylbenzene, tert-	1	-	1	-		-		0.1	X	-	
7440-43-9	Cadmium (Diet)	0.025	0.001	1	-		0.0018	I	0.001	I	1.0x 10^{-5}	A
7440-43-9	Cadmium (Water)				-		0.0018	I	0.0005	I	1.0x 10^{-5}	A
75-15-0	Carbon Disulfide	1	-	1	-		-		0.1	I	0.7	I
56-23-5	Carbon Tetrachloride	1	-	1	0.07	I	6.0 x 10^{-6}	I	0.004	I	0.1	I
12789-03-6	Chlordane	1	0.04	1	0.35	I	0.0001	I	0.0005	I	0.0007	I
143-50-0	Chlordecone (Kepone)	1	0.1	1	10	I	0.0046	C	0.0003	I	-	
106-47-8	Chloroaniline, p-	1	0.1	1	0.2	P	-		0.004	I	-	
108-90-7	Chlorobenzene	1	-	1	-		-		0.02	I	0.05	P
67-66-3	Chloroform	1	-	1	0.031	C	2.3x 10^{-5}	I	0.01	I	0.09765235173824	A
74-87-3	Chloromethane	1	-	1	-		-		-		0.09	I

CAS Number[1]	Compound	GIABS	ABS	RBA	Ingestion SF (mg/kg day)$^{-1}$	Ref[2]	Inhalation Unit Risk ($\mu g/m^3$)$^{-1}$	Ref[2]	Chronic RfD (mg/kg day)	Ref[2]	Chronic RfC (mg/m^3)	Ref[2]
91-58-7	Chloronaphthalene, Beta-	1	0.13	1	-		-		0.08	I	-	
95-57-8	Chlorophenol, 2-	1	-	1	-		-		0.005	I	-	
16065-83-1	Chromium(III), Insoluble Salts	0.013	-	1	-		-		1.5	I	-	
18540-29-9	Chromium(VI)	0.025	-	1	0.5	J	0.084	I	0.003	I	0.0001	I
218-01-9	Chrysene[3]	1	0.13	1	0.0073	S	0.000011	C	-		-	
7440-50-8	Copper	1	-	1	-		-		0.04	H	-	
108-39-4	Cresol, m-	1	0.1	1	-		-		0.05	I	0.6	C
95-48-7	Cresol, o-	1	0.1	1	-		-		0.05	I	0.6	C
106-44-5	Cresol, p-	1	0.1	1	-		-		0.1	A	0.6	C
98-82-8	Cumene	1	-	1	-		-		0.1	I	0.4	I
57-12-5	Cyanide (CN-)[5]	1	-	1	-		-		0.0006	I	0.0008	S
110-82-7	Cyclohexane	1	-	1	-		-		-		6	I
72-54-8	DDD	1	0.1	1	0.24	I	0.000069	C	-		-	
72-55-9	DDE, p,p'-	1	-	1	0.34	I	0.000097	C	-		-	
50-29-3	DDT	1	0.03	1	0.34	I	0.000097	I	0.0005	I	-	
53-70-3	Dibenz[a,h]anthracene[3]	1	0.13	1	7.3	S	0.0012	C	-		-	
132-64-9	Dibenzofuran	1	0.03	1	-		-		0.001	X	-	
124-48-1	Dibromochloromethane	1	-	1	0.084	I	-		0.02	I	-	
106-93-4	Dibromoethane, 1,2-	1	-	1	2	I	0.0006	I	0.009	I	0.009	I
74-95-3	Dibromomethane (Methylene Bromide)	1	-	1	-		-		-		0.004	X
84-74-2	Dibutyl Phthalate	1	0.1	1	-		-		0.1	I	-	
95-50-1	Dichlorobenzene, 1,2-	1	-	1	-		-		0.09	I	0.2	H
541-73-1	Dichlorobenzene, 1,3-[6]	1	-	1	-		-		0.09	S	0.2	S
106-46-7	Dichlorobenzene, 1,4-	1	-	1	0.0054	C	0.000011	C	0.07	A	0.8	I
91-94-1	Dichlorobenzidine, 3,3'-	1	0.1	1	0.45	I	0.00034	C	-		-	
75-71-8	Dichlorodifluoromethane	1	-	1	-		-		0.2	I	0.1	X
75-34-3	Dichloroethane, 1,1-	1	-	1	0.0057	C	1.6×10^{-6}	C	0.2	P	-	
107-06-2	Dichloroethane, 1,2-	1	-	1	0.091	I	0.000026	I	0.006	X	0.007	P
75-35-4	Dichloroethylene, 1,1-	1	-	1	-		-		0.05	I	0.2	I
156-59-2	Dichloroethylene, 1,2-cis-	1	-	1	-		-		0.002	I	-	
156-60-5	Dichloroethylene, 1,2-trans-	1	-	1	-		-		0.02	I	-	
120-83-2	Dichlorophenol, 2,4-	1	0.1	1	-		-		0.003	I	-	
94-75-7	Dichlorophenoxy Acetic Acid, 2,4-	1	0.05	1	-		-		0.01	I	-	
78-87-5	Dichloropropane, 1,2-	1	-	1	0.036	C	$1.0x\ 10^{-5}$	C	0.09	A	0.004	I
542-75-6	Dichloropropene, 1,3-	1	-	1	0.1	I	4.0×10^{-6}	I	0.03	I	0.02	I
60-57-1	Dieldrin	1	0.1	1	16	I	0.0046	I	0.00005	I	-	
84-66-2	Diethyl Phthalate	1	0.1	1	-		-		0.8	I	-	
105-67-9	Dimethylphenol, 2,4-	1	0.1	1	-		-		0.02	I	-	
131-11-3	Dimethylphthalate[7]	1	0.1	1	-		-		0.8	S	-	
528-29-0	Dinitrobenzene, 1,2-	1	0.1	1	-		-		0.0001	P	-	
99-65-0	Dinitrobenzene, 1,3-	1	0.1	1	-		-		0.0001	I	-	
100-25-4	Dinitrobenzene, 1,4-	1	0.1	1	-		-		0.0001	P	-	
51-28-5	Dinitrophenol, 2,4-	1	0.1	1	-		-		0.002	I	-	
121-14-2	Dinitrotoluene, 2,4-	1	0.102	1	0.31	C	0.000089	C	0.002	I	-	

CAS Number[1]	Compound	GIABS	ABS	RBA	Ingestion SF (mg/kg day)$^{-1}$	Ref[2]	Inhalation Unit Risk (µg/m^3)$^{-1}$	Ref[2]	Chronic RfD (mg/kg day)	Ref[2]	Chronic RfC (mg/m^3)	Ref[2]
606-20-2	Dinitrotoluene, 2,6-	1	0.099	1	1.5	P	-		0.0003	X	-	
35572-78-2	Dinitrotoluene, 2-Amino-4,6-[13]	1	0.006	1	-		-		0.002	S	-	
19406-51-0	Dinitrotoluene, 4-Amino-2,6-[13]	1	0.009	1	-		-		0.002	S	-	
123-91-1	Dioxane, 1,4-	1	-	1	0.1	I	5 x 10^{-6}	I	0.03	I	0.03	I
122-39-4	Diphenylamine	1	0.1	1	-		-		0.025	I	-	
115-29-7	Endosulfan	1	-	1	-		-		0.006	I	-	
72-20-8	Endrin	1	0.1	1	-		-		0.0003	I	-	
75-00-3	Ethyl Chloride	1	-	1	-		-		-		10	I
100-41-4	Ethylbenzene	1	-	1	0.011	C	2.5 x 10^{-6}	C	0.1	I	1	I
107-21-1	Ethylene Glycol	1	0.1	1	-		-		2	I	0.4	C
206-44-0	Fluoranthene	1	0.13	1	-		-		0.04	I	-	
86-73-7	Fluorene	1	0.13	1	-		-		0.04	I	-	
50-00-0	Formaldehyde	1	-	1	-		0.000013	I	0.2	I	0.00982576687116	A
76-44-8	Heptachlor	1	-	1	4.5	I	0.0013	I	0.0005	I	-	
1024-57-3	Heptachlor Epoxide	1	-	1	9.1	I	0.0026	I	0.000013	I	-	
118-74-1	Hexachlorobenzene	1	-	1	1.6	I	0.00046	I	0.0008	I	-	
87-68-3	Hexachlorobutadiene	1	-	1	0.078	I	0.000022	I	0.001	P	-	
319-84-6	Hexachlorocyclohexane, Alpha-	1	0.1	1	6.3	I	0.0018	I	0.008	A	-	
319-85-7	Hexachlorocyclohexane, Beta-	1	0.1	1	1.8	I	0.00053	I	-		-	
58-89-9	Hexachlorocyclohexane, Gamma- (Lindane)	1	0.04	1	1.1	C	0.00031	C	0.0003	I	-	
77-47-4	Hexachlorocyclopentadiene	1	-	1	-		-		0.006	I	0.0002	I
67-72-1	Hexachloroethane	1	-	1	0.04	I	0.000011	C	0.0007	I	0.03	I
121-82-4	Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	1	0.015	1	0.11	I	-		0.003	I	-	
110-54-3	Hexane, N-	1	-	1	-		-		-		0.7	I
591-78-6	Hexanone, 2-	1	-	1	-		-		0.005	I	0.03	I
302-01-2	Hydrazine	1	-	1	3	I	0.0049	I	-		0.00003	P
193-39-5	Indeno[1,2,3-cd]pyrene[3]	1	0.13	1	0.73	S	0.00011	C	-		-	
78-59-1	Isophorone	1	0.1	1	0.00095	I	-		0.2	I	2	C
67-63-0	Isopropanol	1	-	1	-		-		2	P	0.2	P
7439-92-1	Lead and Compounds[8]	1	-	1	-		-		-		-	
7487-94-7	Mercuric Chloride[9]	0.07	-	1	-		-		0.0003	I	0.0003	S
7439-97-6	Mercury (elemental)	1	-	1	-		-		0.00016	C	0.0003	I
67-56-1	Methanol	1	-	1	-		-		2	I	20	I
72-43-5	Methoxychlor	1	0.1	1	-		-		0.005	I	-	
78-93-3	Methyl Ethyl Ketone (2-Butanone)	1	-	1	-		-		0.6	I	5	I
108-10-1	Methyl Isobutyl Ketone (4-methyl-2-pentanone)	1	-	1	-		-		-		3	I
22967-92-6	Methyl Mercury	1	-	1	-		-		0.0001	I	-	
1634-04-4	Methyl tert-Butyl Ether (MTBE)	1	-	1	0.0018	C	2.6 x 10^{-7}	C	-		3	I
75-09-2	Methylene Chloride	1	-	1	0.002	I	1 x 10^{-8}	I	0.006	I	0.6	I
90-12-0	Methylnaphthalene, 1-	1	0.13	1	0.029	P	-		0.07	A	-	
91-57-6	Methylnaphthalene, 2-	1	0.13	1	-		-		0.004	I	-	
91-20-3	Naphthalene	1	0.13	1	-		0.000034	C	0.02	I	0.003	I
7440-02-0	Nickel Soluble Salts	0.04	-	1	-		0.00026	C	0.02	I	0.00009	A
98-95-3	Nitrobenzene	1	-	1	-		0.00004	I	0.002	I	0.009	I

CAS Number[1]	Compound	GIABS	ABS	RBA	Ingestion SF (mg/kg day)$^{-1}$	Ref[2]	Inhalation Unit Risk ($\mu g/m^3$)$^{-1}$	Ref[2]	Chronic RfD (mg/kg day)	Ref[2]	Chronic RfC (mg/m^3)	Ref[2]
55-63-0	Nitroglycerin	1	0.1	1	0.017	P	-		0.0001	P	-	
556-88-7	Nitroguanidine	1	0.1	1	-		-		0.1	I	-	
62-75-9	Nitrosodimethylamine, N-	1	-	1	51	I	0.014	I	8×10^{-6}	P	0.00004	X
621-64-7	Nitroso-di-N-propylamine, N-	1	0.1	1	7	I	0.002	C	-		-	
86-30-6	Nitrosodiphenylamine, N-	1	0.1	1	0.0049	I	2.6×10^{-6}	C	-		-	
99-08-1	Nitrotoluene, m-	1	0.1	1	-		-		0.0001	X	-	
88-72-2	Nitrotoluene, o-	1	-	1	0.22	P	-		0.0009	P	-	
99-99-0	Nitrotoluene, p-	1	0.1	1	0.016	P	-		0.004	P	-	
2691-41-0	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	1	0.006	1	-		-		0.05	I	-	
117-84-0	Octyl Phthalate, di-N-	1	0.1	1	-		-		0.01	P	-	
87-86-5	Pentachlorophenol	1	0.25	1	0.4	I	5.1×10^{-6}	C	0.005	I	-	
78-11-5	Pentaerythritol tetranitrate (PETN)	1	0.1	1	0.004	X	-		0.002	P	-	
1763-23-1	Perfluorooctane Sulfonate (PFOS)[10]	1	0.1	1	-		-		0.00002	W	-	
335-67-1	Perfluorooctanoic Acid (PFOA)[11]	1	0.1	1	0.07	W	-		0.00002	W	-	
85-01-8	Phenanthrene[4]	1	0.13	1	-		-		0.03	S	-	
108-95-2	Phenol	1	0.1	1	-		-		0.3	I	0.2	C
7723-14-0	Phosphorus, White	1	-	1	-		-		0.00002	I	-	
1336-36-3	Polychlorinated Biphenyls[14]	1	0.14	1	2	I	0.00057142857142	I	-		-	
103-65-1	Propyl benzene	1	-	1	-		-		0.1	X	1	X
129-00-0	Pyrene	1	0.13	1	-		-		0.03	I	-	
7782-49-2	Selenium	1	-	1	-		-		0.005	I	0.02	C
7440-22-4	Silver	0.04	-	1	-		-		0.005	I	-	
100-42-5	Styrene	1	-	1	-		-		0.2	I	1	I
1746-01-6	TCDD, 2,3,7,8-[12]	1	0.03	1	130000	C	38	C	7×10^{-10}	I	4×10^{-8}	C
630-20-6	Tetrachloroethane, 1,1,1,2-	1	-	1	0.026	I	7.4×10^{-6}	I	0.03	I	-	
79-34-5	Tetrachloroethane, 1,1,2,2-	1	-	1	0.2	I	0.000058	C	0.02	I	-	
127-18-4	Tetrachloroethylene	1	-	1	0.0021	I	2.6×10^{-7}	I	0.006	I	0.04	I
479-45-8	Tetryl (Trinitrophenylmethylnitramine)	1	0.00065	1	-		-		0.002	P	-	
7440-28-0	Thallium (Soluble Salts)	1	-	1	-		-		$1x\ 10^{-5}$	X	-	
108-88-3	Toluene	1	-	1	-		-		0.08	I	5	I
8001-35-2	Toxaphene	1	0.1	1	1.1	I	0.00032	I	-		-	
76-13-1	Trichloro-1,2,2-trifluoroethane, 1,1,2-	1	-	1	-		-		30	I	30	H
87-61-6	Trichlorobenzene, 1,2,3-	1	-	1	-		-		0.0008	X	-	
120-82-1	Trichlorobenzene, 1,2,4-	1	-	1	0.029	P	-		0.01	I	0.002	P
71-55-6	Trichloroethane, 1,1,1-	1	-	1	-		-		2	I	5	I
79-00-5	Trichloroethane, 1,1,2-	1	-	1	0.057	I	0.000016	I	0.004	I	0.0002	X
79-01-6	Trichloroethylene	1	-	1	0.046	I	4.1×10^{-6}	I	0.0005	I	0.002	I
75-69-4	Trichlorofluoromethane	1	-	1	-		-		0.3	I	-	
95-95-4	Trichlorophenol, 2,4,5-	1	0.1	1	-		-		0.1	I	-	
88-06-2	Trichlorophenol, 2,4,6-	1	0.1	1	0.011	I	3.1×10^{-6}	I	0.001	P	-	
93-76-5	Trichlorophenoxyacetic Acid, 2,4,5-	1	0.1	1	-		-		0.01	I	-	
93-72-1	Trichlorophenoxypropionic acid, -2,4,5	1	0.1	1	-		-		0.008	I	-	
96-18-4	Trichloropropane, 1,2,3-	1	-	1	30	I	-		0.004	I	0.0003	I
95-63-6	Trimethylbenzene, 1,2,4-	1	-	1	-		-		-		0.007	P

CAS Number[1]	Compound	GIABS	ABS	RBA	Ingestion SF (mg/kg day)$^{-1}$	Ref[2]	Inhalation Unit Risk (µg/m^3)$^{-1}$	Ref[2]	Chronic RfD (mg/kg day)	Ref[2]	Chronic RfC (mg/m^3)	Ref[2]
108-67-8	Trimethylbenzene, 1,3,5-	1	-	1	-		-		0.01	X	-	
688-73-3	Tri-n-butyltin	1	-	1	-		-		0.0003	A	-	
99-35-4	Trinitrobenzene, 1,3,5-	1	0.019	1	-		-		0.03	I	-	
118-96-7	Trinitrotoluene, 2,4,6-	1	0.032	1	0.03	I	-		0.0005	I	-	
7440-62-2	Vanadium and Compounds	0.026	-	1	-		-		0.00504	X	0.0001	A
108-05-4	Vinyl Acetate	1	-	1	-		-		1	H	0.2	I
75-01-4	Vinyl Chloride	1	-	1	0.72	I	4.4×10^{-6}	I	0.003	I	0.1	I
1330-20-7	Xylenes	1	-	1	-		-		0.2	I	0.1	I
7440-66-6	Zinc and Compounds	1	-	1	-		-		0.3	I	-	

[1] "CAS Number" means the Chemical Abstract Service (CAS) registry number uniquely assigned to chemicals by the American Chemical Society and recorded in the CAS Registry System

[2] Reference source for data; I= Integrated Risk Information System; P= Provisional Peer Reviewed Toxicity Values; A= Agency for Toxic Substances and Disease Registry; C= California Environmental Protection Agency (EPA); X=Appendix Provisional Peer Reviewed Toxicity Values Screen; H=EPA's Health Effects Assessment Summary Tables; J=New Jersey; S=Surrogate Compound; W= EPA Office of Water

[3] Polycyclic aromatic hydrocarbons (PAH) ingestion slope factors are determined using Benzo[a]pyrene and Toxicity Equivalence Factors (TEFs) as described in the Risk Assessment Procedures Manual

[4] Pyrene is a toxicity surrogate for acenaphthylene, benzo(g,h,i)perylene, and phenanthrene

[5] Cyanide expressed as free, or physiologically available cyanide; The IRIS RfC for "Hydrogen Cyanide" is used as a surrogate for "Cyanide (CN-)".

[6] 1,2-dichlorobenzene is a toxicity surrogate for 1,3-dichlorobenzene

[7] Diethylphthalate is a toxicity surrogate for dimethylphthalate

[8] Lead cleanup levels are based on land use; for residential land use, the soil cleanup level is 400 mg/kg

[9] Elemental mercury is a toxicity surrogate for mercuric chloride

[10] Toxicity is given in EPA's Health Effects Support Document for Perfluorooctane Sulfonate (PFOS) 2016.

[11] Toxicity is given in EPA's Health Effects Support Document for Perfluorooctanoic Acid (PFOA) 2016.

[12] The cleanup level in 18 AAC 75.341(c) Table B1 is for 2,3,7,8-Tetrachlorordibenzo-p-Dioxin (TCDD) only; all cleanup levels for polychlorinated dibenzo-p-dioxin and polychlorinated dibenzofuran congeners must be determined on a site-specific basis.

[13] The IRIS oral RfD for 2,4-Dinitrotoluene is used as a surrogate for 2-Amino-4,6-Dinitrotoluene and 4-Amino-2,6-Dinitrotoluene.

[14] For unrestricted land use, the cleanup level for polychlorinated biphenyls (PCBs) is 1 mg/kg.

Table 7 Organic and Inorganic Chemical Specific Parameters

CAS Number[1]	Compound	VOC	D_{ia} (cm^2/s)	D_{iw} (cm^2/s)	Solubility (mg/L)	K_d (cm^3/g)	K_{oc} (cm^3/g)	H' (unitless)	MW (g/mol)	FA	Kp (cm/h)	Melting Point (°C)
83-32-9	Acenaphthene	Yes	0.0506143	8.33×10^{-6}	3.9	5.027	5027	0.00752248569092	154.21	1	0.086	93.4
208-96-8	Acenaphthylene	Yes	0.0449596	6.9822×10^{-6}	16.1	5.027	5027	0.00466067048242	152.2	1	0.0911	92.5
67-64-1	Acetone	Yes	0.1059215	0.0000115	1000000	0.002364	2.364	0.00143090760425	58.081	1	0.000512	-98.3
309-00-2	Aldrin	Yes	0.0228116	5.8402×10^{-6}	0.017	82.02	82020	0.00179885527391	364.92	1	-	240
7790-98-9	Ammonium Perchlorate	No	-	-	245000	0	-	-	117.49	1	0.001	-
120-12-7	Anthracene	Yes	0.0389732	7.8523×10^{-6}	0.0434	16.36	16360	0.00227309893704	178.24	1	0.142	215
7440-36-0	Antimony (metallic)	No	-	-	-	45	-	-	124.77	1	0.001	630.628
7440-38-2	Arsenic, Inorganic	No	-	-	-	29	-	-	77.946	1	0.001	270
7440-39-3	Barium	No	-	-	-	41	-	-	139.36	1	0.001	727
56-55-3	Benz[a]anthracene	Yes	0.0261138	6.7495×10^{-6}	0.0094	176.9	176900	0.00049059689288	228.3	1	-	84
100-52-7	Benzaldehyde	Yes	0.074393	9.4627×10^{-6}	6950	0.01109	11.09	0.00109157808667	106.13	1	0.00383	-26
71-43-2	Benzene	Yes	0.089534	0.0000103	1790	0.1458	145.8	0.22690106295993	78.115	1	0.0149	5.5
50-32-8	Benzo[a]pyrene	No	0.0475831	5.5597×10^{-6}	0.00162	587.4	587400	0.000018683565	252.32	1	-	176.5
205-99-2	Benzo[b]fluoranthene	No	0.0475831	5.5597×10^{-6}	0.0015	599.4	599400	0.00002686017988	252.32	1	-	168
191-24-2	Benzo[g,h,i]perylene	No	0.0447842	5.2327×10^{-6}	0.00026	1951	1951000	0.00001353229762	276.34	0.7	-	278
207-08-9	Benzo[k]fluoranthene	No	0.0475831	5.5597×10^{-6}	0.0008	587.4	587400	0.00002387571545	252.32	0.9	-	217
65-85-0	Benzoic Acid	No	0.0701939	9.7868×10^{-6}	3400	0.0006	0.6	$1.5576451349141 \times 10^{-6}$	122.12	1	0.00565	122.4
100-51-6	Benzyl Alcohol	No	0.0731186	9.3665×10^{-6}	42900	0.02146	21.46	0.00001377759607	108.14	1	0.00209	-15.2
7440-41-7	Beryllium and compounds	No	-	-	-	790	-	-	11.028	1	0.001	986
111-44-4	Bis(2-chloroethyl)ether	Yes	0.0567192	8.707×10^{-6}	17200	0.03221	32.21	0.00069501226492	143.01	1	0.00178	-51.9
117-81-7	Bis(2-ethylhexyl)phthalate	No	0.0173403	4.1807×10^{-6}	0.27	119.6	119600	0.00001103843008	390.57	0.8	-	-55
108-86-1	Bromobenzene	Yes	0.0537132	9.3004×10^{-6}	446	0.2339	233.9	0.10098119378577	157.01	1	0.02	-30.6
75-27-4	Bromodichloromethane	Yes	0.0562629	0.0000107	3032	0.03182	31.82	0.08667211774325	163.83	1	0.00402	-57
75-25-2	Bromoform	Yes	0.0357324	0.0000104	3100	0.03182	31.82	0.02187244480784	252.73	1	0.00235	8
74-83-9	Bromomethane	Yes	0.1004976	0.0000135	15200	0.01322	13.22	0.30008176614881	94.939	1	0.00284	-93.7
106-99-0	Butadiene, 1,3-	Yes	0.1003488	0.0000103	735	0.0396	39.6	3.00899427636958	54.092	1	0.0164	-108.9
71-36-3	Butanol, N-	Yes	0.0900387	0.0000101	63200	0.003471	3.471	0.00036017988552	74.124	1	0.00231	-89.8
85-68-7	Butyl Benzyl Phthalate	No	0.0208319	5.1733×10^{-6}	2.69	7.155	7155	0.00005151267375	312.37	0.9	0.0385	-35
104-51-8	Butylbenzene, n-	Yes	0.0527732	7.3335×10^{-6}	11.8	1.482	1482	0.6500408830744	134.22	1	-	-87.9
135-98-8	Butylbenzene, sec-	Yes	0.0527928	7.3371×10^{-6}	17.6	1.331	1331	0.71954210956663	134.22	1	-	-82.7
98-06-6	Butylbenzene, tert-	Yes	0.0529525	7.3662×10^{-6}	29.5	1.001	1001	0.53965658217498	134.22	1	0.149	-57.8
7440-43-9	Cadmium	No	-	-	-	75	-	-	112.4	1	0.001	321
75-15-0	Carbon Disulfide	Yes	0.1064373	0.000013	2160	0.02173	21.73	0.58871627146361	76.139	1	0.0114	-111.5
56-23-5	Carbon Tetrachloride	Yes	0.0571435	9.7849×10^{-6}	793	0.04389	43.89	1.12837285363859	153.82	1	0.0163	-23
12789-03-6	Chlordane	Yes	0.021493	5.4477×10^{-6}	0.056	67.54	67540	0.00198691741618	409.78	0.7	0.107	132.97
143-50-0	Chlordecone (Kepone)	No	0.019647	4.9081×10^{-6}	2.7	17.5	17500	$2.1995094031071 \times 10^{-6}$	490.64	0.8	0.0109	350
106-47-8	Chloroaniline, p-	No	0.0703847	0.0000103	3900	0.1127	112.7	0.00004742436631	127.57	1	0.00496	72.5
108-90-7	Chlorobenzene	Yes	0.0721306	9.4765×10^{-6}	498	0.2339	233.9	0.12714636140637	112.56	1	0.0282	-45.2
67-66-3	Chloroform	Yes	0.0769197	0.0000109	7950	0.03182	31.82	0.1500408830744	119.38	1	0.00683	-63.6
74-87-3	Chloromethane	Yes	0.1239651	0.0000136	5320	0.01322	13.22	0.36058871627146	50.488	1	0.00328	-97.7
91-58-7	Chloronaphthalene, Beta-	Yes	0.0446914	7.7301×10^{-6}	11.7	2.478	2478	0.0130825838103	162.62	1	0.0749	61

CAS Number[1]	Compound	VOC	D_{ia} (cm^2/s)	D_{iw} (cm^2/s)	Solubility (mg/L)	K_d (cm^3/g)	K_{oc} (cm^3/g)	H' (unitless)	MW (g/mol)	FA	Kp (cm/h)	Melting Point (°C)
95-57-8	Chlorophenol, 2-	Yes	0.0661175	9.4784×10^{-6}	11300	0.388	388	0.00045789043336	128.56	1	0.00799	9.8
16065-83-1	Chromium(III), Insoluble Salts	No	-	-	-	1800000	-	-	52	1	0.001	-
18540-29-9	Chromium(VI)	No	-	-	1690000	19	-	-	52	1	0.002	-
218-01-9	Chrysene	No	0.0261138	6.7495×10^{-6}	0.002	180.5	180500	0.00021381847914	228.3	1	-	258.2
7440-50-8	Copper	No	-	-	-	35	-	-	63.546	1	0.001	1084.62
108-39-4	Cresol, m-	No	0.0728721	9.3232×10^{-6}	22700	0.3004	300.4	0.00003499591169	108.14	1	0.00777	11.8
95-48-7	Cresol, o-	No	0.072835	9.3168×10^{-6}	25900	0.3065	306.5	0.00004905968928	108.14	1	0.00766	29.8
106-44-5	Cresol, p-	No	0.0723938	9.2397×10^{-6}	21500	0.3004	300.4	0.0000408830744	108.14	1	0.00754	35.5
98-82-8	Cumene	Yes	0.0603044	7.8566×10^{-6}	61.3	0.6978	697.8	0.47015535568274	120.2	1	0.0897	-96
57-12-5	Cyanide (CN-)	Yes	0.2109549	0.0000246	95400	9.9	-	0.00415	26.018	1	0.001	-
110-82-7	Cyclohexane	Yes	0.0799729	9.1077×10^{-6}	55	0.1458	145.8	6.13246116107931	84.163	1	0.102	6.6
72-54-8	DDD	No	0.0406077	4.7447×10^{-6}	0.09	117.5	117500	0.00026982829108	320.05	0.8	0.251	109.5
72-55-9	DDE, p,p'-	Yes	0.0229959	5.8592×10^{-6}	0.04	117.5	117500	0.00170073589533	318.03	0.8	-	89
50-29-3	DDT	No	0.037933	4.4322×10^{-6}	0.0055	168.6	168600	0.00034014717906	354.49	0.7	-	108.5
53-70-3	Dibenz[a,h]anthracene	No	0.0445672	5.2073×10^{-6}	0.00249	1912	1912000	$5.7645134914145 \times 10^{-6}$	278.36	0.6	-	269.5
132-64-9	Dibenzofuran	Yes	0.0650663	7.3773×10^{-6}	3.1	9.161	9161	0.00870809484873	168.2	1	0.0975	86.5
124-48-1	Dibromochloromethane	Yes	0.0366356	0.0000106	2700	0.03182	31.82	0.03201144726083	208.28	1	0.00289	-20
106-93-4	Dibromoethane, 1,2-	Yes	0.0430348	0.0000104	3910	0.0396	39.6	0.02657399836467	187.86	1	0.00278	9.9
74-95-3	Dibromomethane (Methylene Bromide)	Yes	0.0551373	0.0000119	11900	0.02173	21.73	0.03360588716271	173.84	1	0.00223	-52.5
84-74-2	Dibutyl Phthalate	No	0.0214362	5.3255×10^{-6}	11.2	1.157	1157	0.00007399836467	278.35	0.9	0.042	-35
95-50-1	Dichlorobenzene, 1,2-	Yes	0.0561703	8.9213×10^{-6}	156	0.3829	382.9	0.07849550286181	147	1	0.0446	-16.7
541-73-1	Dichlorobenzene, 1,3-	Yes	0.0558361	8.8494×10^{-6}	125	0.3753	375.3	0.10752248569092	147	1	0.052	-24.8
106-46-7	Dichlorobenzene, 1,4-	Yes	0.0550429	8.6797×10^{-6}	81.3	0.3753	375.3	0.09852820932134	147	1	0.0453	52.09
91-94-1	Dichlorobenzidine, 3,3'-	No	0.0474815	5.5478×10^{-6}	3.1	3.19	3190	$1.1610793131643 \times 10^{-9}$	253.13	1	0.0128	132
75-71-8	Dichlorodifluoromethane	Yes	0.0760293	0.0000108	280	0.04389	43.89	14.022894521668	120.91	1	0.00895	-158
75-34-3	Dichloroethane, 1,1-	Yes	0.0836446	0.0000106	5040	0.03182	31.82	0.22976287816843	98.96	1	0.00675	-96.9
107-06-2	Dichloroethane, 1,2-	Yes	0.0857221	0.000011	8600	0.0396	39.6	0.04824202780049	98.96	1	0.0042	-35.5
75-35-4	Dichloroethylene, 1,1-	Yes	0.0863107	0.000011	2420	0.03182	31.82	1.0670482420278	96.944	1	0.0117	-122.5
156-59-2	Dichloroethylene, 1,2-cis-	Yes	0.0884056	0.0000113	6410	0.0396	39.6	0.16680294358135	96.944	1	0.011	-57
156-60-5	Dichloroethylene, 1,2-trans-	Yes	0.0876094	0.0000112	4520	0.0396	39.6	0.38348323793949	96.944	1	0.011	-49.8
120-83-2	Dichlorophenol, 2,4-	No	0.0485768	8.6787×10^{-6}	5550	0.147	147	0.0001753883892	163	1	0.0206	45
94-75-7	Dichlorophenoxy Acetic Acid, 2,4-	No	0.0279179	7.3445×10^{-6}	677	0.02963	29.63	$1.4472608340147 \times 10^{-6}$	221.04	1	0.00664	140.5
78-87-5	Dichloropropane, 1,2-	Yes	0.0733402	9.7252×10^{-6}	2800	0.0607	60.7	0.11529026982829	112.99	1	0.00753	-100
542-75-6	Dichloropropene, 1,3-	Yes	0.0762725	0.0000101	2800	0.07217	72.17	0.14513491414554	110.97	1	0.00834	-50
60-57-1	Dieldrin	No	0.0232865	6.0062×10^{-6}	0.195	20.09	20090	0.00040883074407	380.91	0.8	0.0326	175.5
84-66-2	Diethyl Phthalate	No	0.0260741	6.7227×10^{-6}	1080	0.1049	104.9	0.00002493867538	222.24	1	0.0036	-40.5
105-67-9	Dimethylphenol, 2,4-	No	0.0622451	8.314×10^{-6}	7870	0.4918	491.8	0.00003887980376	122.17	1	0.0109	24.5
131-11-3	Dimethylphthalate	No	0.0299117	7.1412×10^{-6}	4000	0.03159	31.59	$8.0539656582175 \times 10^{-6}$	194.19	1	0.00147	5.5
528-29-0	Dinitrobenzene, 1,2-	No	0.0447176	8.2538×10^{-6}	133	0.3588	358.8	$2.1790678659035 \times 10^{-6}$	168.11	1	0.00237	118.5
99-65-0	Dinitrobenzene, 1,3-	No	0.0484987	9.2109×10^{-6}	533	0.3516	351.6	$2.0032706459525 \times 10^{-6}$	168.11	1	0.00174	90
100-25-4	Dinitrobenzene, 1,4-	No	0.0491668	9.3849×10^{-6}	69	0.3516	351.6	$3.4300899427637 \times 10^{-6}$	168.11	1	0.00167	174
51-28-5	Dinitrophenol, 2,4-	No	0.0406699	9.0756×10^{-6}	2790	0.4608	460.8	$3.5159443990188 \times 10^{-6}$	184.11	1	0.00187	115.5
121-14-2	Dinitrotoluene, 2,4-	No	0.0375115	7.8982×10^{-6}	200	0.5756	575.6	$2.2076860179885 \times 10^{-6}$	182.14	1	0.00308	71

CAS Number[1]	Compound	VOC	D_{ia} (cm^2/s)	D_{iw} (cm^2/s)	Solubility (mg/L)	K_d (cm^3/g)	K_{oc} (cm^3/g)	H' (unitless)	MW (g/mol)	FA	Kp (cm/h)	Melting Point (°C)
606-20-2	Dinitrotoluene, 2,6-	No	0.0370256	7.7629×10^{-6}	182	0.5874	587.4	0.00003053965658	182.14	1	0.0037	66
35572-78-2	Dinitrotoluene, 2-Amino-4,6-	No	0.0560905	6.5537×10^{-6}	1220	0.283	283	$1.3368765331152 \times 10^{-9}$	197.15	1	0.00204	174.5
19406-51-0	Dinitrotoluene, 4-Amino-2,6-	No	0.0560905	6.5537×10^{-6}	1220	0.283	283	$1.3368765331152 \times 10^{-9}$	197.15	1	0.00204	171
123-91-1	Dioxane, 1,4-	Yes	0.0873739	0.0000105	1000000	0.002633	2.633	0.00019623875715	88.107	1	0.000332	11.8
122-39-4	Diphenylamine	No	0.0417056	7.628×10^{-6}	53	0.8258	825.8	0.00010997547015	169.23	1	0.0373	52.9
115-29-7	Endosulfan	Yes	0.0224845	5.7629×10^{-6}	0.325	6.761	6761	0.00265739983646	406.93	0.9	0.00286	106
72-20-8	Endrin	No	0.0361581	4.2248×10^{-6}	0.25	20.09	20090	0.00026001635322	380.91	0.8	0.0326	226
75-00-3	Ethyl Chloride	Yes	0.1037597	0.0000116	6710	0.02173	21.73	0.45380212591986	64.515	1	0.00607	-138.7
100-41-4	Ethylbenzene	Yes	0.0684652	8.4558×10^{-6}	169	0.4461	446.1	0.3221586263287	106.17	1	0.0493	-94.9
107-21-1	Ethylene Glycol	No	0.116925	0.0000136	1000000	0.001	1	2.453×10^{-6}	62.069	1	0.0000877	-13
206-44-0	Fluoranthene	No	0.0275957	7.1827×10^{-6}	0.26	55.45	55450	0.00036222403924	202.26	1	-	107.8
86-73-7	Fluorene	Yes	0.0439743	7.889×10^{-6}	1.69	9.16	9160	0.00393295175797	166.22	1	0.11	114.8
50-00-0	Formaldehyde	Yes	0.1670871	0.0000174	400000	0.001	1	0.00001377759607	30.026	1	0.00182	-92
76-44-8	Heptachlor	Yes	0.0223441	5.6959×10^{-6}	0.18	41.26	41260	0.01201962387571	373.32	0.8	0.143	95.5
1024-57-3	Heptachlor Epoxide	Yes	0.0240006	6.2475×10^{-6}	0.2	10.11	10110	0.00085854456255	389.32	0.8	0.0209	160
118-74-1	Hexachlorobenzene	Yes	0.0289745	7.8497×10^{-6}	0.0062	6.195	6195	0.06950122649223	284.78	0.9	-	231.8
87-68-3	Hexachlorobutadiene	Yes	0.0267445	7.0264×10^{-6}	3.2	0.8452	845.2	0.42109566639411	260.76	0.9	0.081	-21
319-84-6	Hexachlorocyclohexane, Alpha-	No	0.043284	5.0574×10^{-6}	2	2.807	2807	0.00027391659852	290.83	0.9	0.0206	112.5
319-85-7	Hexachlorocyclohexane, Beta-	No	0.0276672	7.3955×10^{-6}	0.24	2.807	2807	0.00001798855273	290.83	0.9	0.0206	112.5
58-89-9	Hexachlorocyclohexane, Gamma- (Lindane)	No	0.043284	5.0574×10^{-6}	7.3	2.807	2807	0.00021013900245	290.83	0.9	0.0206	112.5
77-47-4	Hexachlorocyclopentadiene	Yes	0.0272382	7.217×10^{-6}	1.8	1.404	1404	1.10384300899428	272.77	0.9	0.103	-9
67-72-1	Hexachloroethane	Yes	0.0320938	8.8904×10^{-6}	50	0.1968	196.8	0.15903515944399	236.74	1	0.0415	187
121-82-4	Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	No	0.0311541	8.4989×10^{-6}	59.7	0.08907	89.07	$8.2174979558462 \times 10^{-10}$	222.12	1	0.000336	205.5
110-54-3	Hexane, N-	Yes	0.0731078	8.1657×10^{-6}	9.5	0.1315	131.5	73.5895339329518	86.178	1	0.201	-95.3
591-78-6	Hexanone, 2-	Yes	0.0703564	8.4404×10^{-6}	17200	0.01498	14.98	0.00381030253475	100.16	1	0.00355	-55.5
302-01-2	Hydrazine[3]	Yes	0.1733034	0.000019	1000000	0.002	2	0.000025	32.045	1	0.0000436	2
193-39-5	Indeno[1,2,3-cd]pyrene	No	0.0447842	5.2327×10^{-6}	0.00019	1951	1951000	0.00001422730989	276.34	0.6	-	163.6
78-59-1	Isophorone	No	0.0525048	7.5296×10^{-6}	12000	0.06515	65.15	0.00027146361406	138.21	1	0.00354	-8.1
67-63-0	Isopropanol	Yes	0.1032261	0.0000112	1000000	0.00153	1.53	0.00033115290269	60.097	1	0.000778	-89.5
7439-92-1	Lead and Compounds	No	-	-	-	900	-	-	207.2	1	0.0001	327.5
7487-94-7	Mercuric Chloride	No	-	-	69000	52	-	-	271.5	1	0.001	277
7439-97-6	Mercury (elemental)	Yes	0.0307	6.3×10^{-6}	0.06	52	-	0.352	200.59	1	0.001	-38.8
67-56-1	Methanol	Yes	0.1582741	0.0000165	1000000	0.001	1	0.00018601798855	32.042	1	0.000319	-97.6
72-43-5	Methoxychlor	No	0.0220849	5.5926×10^{-6}	0.1	26.89	26890	$8.2992641046606 \times 10^{-6}$	345.66	0.8	0.0428	87
78-93-3	Methyl Ethyl Ketone (2-Butanone)	Yes	0.0914462	0.0000102	223000	0.00451	4.51	0.00232624693376	72.108	1	0.000962	-86.6
108-10-1	Methyl Isobutyl Ketone (4-methyl-2-pentanone)	Yes	0.0697797	8.3477×10^{-6}	19000	0.0126	12.6	0.00564186426819	100.16	1	0.00319	-84
22967-92-6	Methyl Mercury[4]	No	-	-	-	7000	-	-	216.6326	1	0.001	-
1634-04-4	Methyl tert-Butyl Ether (MTBE)	Yes	0.0752672	8.5905×10^{-6}	51000	0.01156	11.56	0.02399836467702	88.151	1	0.00211	-108.6
75-09-2	Methylene Chloride	Yes	0.0999362	0.0000125	13000	0.02173	21.73	0.13286999182338	84.933	1	0.00354	-95.1
90-12-0	Methylnaphthalene, 1-	Yes	0.0527705	7.8477×10^{-6}	25.8	2.528	2528	0.02101390024529	142.2	1	0.0931	34
91-57-6	Methylnaphthalene, 2-	Yes	0.0524319	7.7811×10^{-6}	24.6	2.478	2478	0.02117743254292	142.2	1	0.0917	34.4
91-20-3	Naphthalene	Yes	0.0604994	8.377×10^{-6}	31	1.544	1544	0.01798855273916	128.18	1	0.0466	80.2
7440-02-0	Nickel Soluble Salts	No	-	-	-	65	-	-	58.71	1	0.0002	1455

CAS Number[1]	Compound	VOC	D_{ia} (cm^2/s)	D_{iw} (cm^2/s)	Solubility (mg/L)	K_d (cm^3/g)	K_{oc} (cm^3/g)	H' (unitless)	MW (g/mol)	FA	Kp (cm/h)	Melting Point (°C)
98-95-3	Nitrobenzene	Yes	0.068054	9.4495×10^{-6}	2090	0.2264	226.4	0.00098119378577	123.11	1	0.00541	5.7
55-63-0	Nitroglycerin	No	0.029015	7.7428×10^{-6}	1380	0.1158	115.8	$3.5404742436631 \times 10^{-6}$	227.09	1	0.000994	13.5
556-88-7	Nitroguanidine	No	0.0996937	0.0000142	4400	0.02065	20.65	$1.8192968111202 \times 10^{-14}$	104.07	1	0.000105	239
62-75-9	Nitrosodimethylamine, N-	Yes	0.0987674	0.0000115	1000000	0.02279	22.79	0.00007440719542	74.083	1	0.000251	-39.07
621-64-7	Nitroso-di-N-propylamine, N-	No	0.0564399	7.758×10^{-6}	13000	0.2754	275.4	0.00021995094031	130.19	1	0.00233	6.81
86-30-6	Nitrosodiphenylamine, N-	No	0.0558866	6.5299×10^{-6}	35	2.632	2632	0.00004946852003	198.23	1	0.0145	66.5
99-08-1	Nitrotoluene, m-	No	0.058686	8.6541×10^{-6}	500	0.3632	363.2	0.00038021259198	137.14	1	0.0113	15.5
88-72-2	Nitrotoluene, o-	Yes	0.0587535	8.6675×10^{-6}	650	0.3706	370.6	0.00051103843008	137.14	1	0.00899	-10
99-99-0	Nitrotoluene, p-	No	0.0574432	8.4083×10^{-6}	442	0.3632	363.2	0.00023017170891	137.14	1	0.01	51.6
2691-41-0	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	No	0.0427631	4.9965×10^{-6}	5	0.5316	531.6	$3.5445625511038 \times 10^{-8}$	296.16	1	0.0000436	286
117-84-0	Octyl Phthalate, di-N-	No	0.0355594	4.1548×10^{-6}	0.022	140.8	140800	0.00010506950122	390.57	0	-	-4
87-86-5	Pentachlorophenol	No	0.0295197	8.0121×10^{-6}	14	0.592	592	$1.0016353229762 \times 10^{-6}$	266.34	0.9	0.127	174
78-11-5	Pentaerythritol tetranitrate (PETN)	No	0.025756	6.7697×10^{-6}	43	0.6479	647.9	$5.3965658217498 \times 10^{-8}$	316.14	1	0.00101	140.5
1763-23-1	Perfluorooctane Sulfonate (PFOS)[5]	No	0.0207478	5.2533×10^{-6}	680	0.3715	371.5	-	500.13	0	-	51.9
335-67-1	Perfluorooctanoic Acid (PFOA)[5]	No	0.02257	5.7947×10^{-6}	9500	0.1148	114.8	-	414.07	0	-	55
85-01-8	Phenanthrene	Yes	0.0344784	6.6897×10^{-6}	1.15	16.69	16690	0.00172935404742	178.24	1	0.144	99.2
108-95-2	Phenol	No	0.0833983	0.0000103	82800	0.1872	187.2	0.00001361406377	94.114	1	0.00434	40.9
7723-14-0	Phosphorus, White	Yes	0.2193655	0.0000277	3	3.5	1122	0.086	123.895	1	0.001	44.15
1336-36-3	Polychlorinated Biphenyls	Yes	0.0243397	6.2671×10^{-6}	0.7	78.1	78100	0.01696647587898	291.99	0.7	-	122.32
103-65-1	Propyl benzene	Yes	0.0601558	7.831×10^{-6}	52.2	0.8131	813.1	0.42927228127555	120.2	1	0.0939	-99.5
129-00-0	Pyrene	Yes	0.0277873	7.2479×10^{-6}	0.135	54.34	54340	0.00048650858544	202.26	1	0.201	151.2
7782-49-2	Selenium	No	-	-	-	5	-	-	78.96	1	0.001	221
7440-22-4	Silver	No	-	-	-	8.3	-	-	107.87	1	0.0006	961.78
100-42-5	Styrene	Yes	0.071114	8.7838×10^{-6}	310	0.4461	446.1	0.11242845461978	104.15	1	0.0372	-31
1746-01-6	TCDD, 2,3,7,8-	Yes	0.0470278	6.7568×10^{-6}	0.0002	249.1	249100	0.00204415372035	321.98	0.5	-	305
630-20-6	Tetrachloroethane, 1,1,1,2-	Yes	0.0481761	9.0977×10^{-6}	1070	0.08603	86.03	0.10220768601798	167.85	1	0.0159	-70.2
79-34-5	Tetrachloroethane, 1,1,2,2-	Yes	0.0489206	9.2902×10^{-6}	2830	0.09494	94.94	0.01500408830744	167.85	1	0.00694	-43.8
127-18-4	Tetrachloroethylene	Yes	0.0504664	9.4551×10^{-6}	206	0.09494	94.94	0.72363041700735	165.83	1	0.0334	-22.3
479-45-8	Tetryl (Trinitrophenylmethylnitramine)	No	0.0255626	6.6672×10^{-6}	74	4.605	4605	$1.107931316435 \times 10^{-7}$	287.15	1	0.000474	131.5
7440-28-0	Thallium (Soluble Salts)	No	-	-	-	71	-	-	205.38	1	0.001	303.5
108-88-3	Toluene	Yes	0.0778039	9.2045×10^{-6}	526	0.2339	233.9	0.27146361406377	92.142	1	0.0311	-94.9
8001-35-2	Toxaphene	No	0.032439	3.7902×10^{-6}	0.55	77.2	77200	0.00024529844644	448.26	0.8	-	65
76-13-1	Trichloro-1,2,2-trifluoroethane, 1,1,2-	Yes	0.0375658	8.592×10^{-6}	170	0.1968	196.8	21.5044971381848	187.38	1	0.0175	-35
87-61-6	Trichlorobenzene, 1,2,3-	Yes	0.03953	8.3836×10^{-6}	18	1.383	1383	0.05110384300899	181.45	1	0.0738	53.5
120-82-1	Trichlorobenzene, 1,2,4-	Yes	0.0395992	8.4033×10^{-6}	49	1.356	1356	0.05805396565821	181.45	1	0.0705	17
71-55-6	Trichloroethane, 1,1,1-	Yes	0.0648174	9.599×10^{-6}	1290	0.04389	43.89	0.70318887980376	133.41	1	0.0126	-30.4
79-00-5	Trichloroethane, 1,1,2-	Yes	0.0668904	0.00001	4590	0.0607	60.7	0.03368765331152	133.41	1	0.00504	-36.6
79-01-6	Trichloroethylene	Yes	0.0686618	0.0000102	1280	0.0607	60.7	0.40269828291087	131.39	1	0.0116	-84.7
75-69-4	Trichlorofluoromethane	Yes	0.065356	0.00001	1100	0.04389	43.89	3.96565821749796	137.37	1	0.0127	-111.1
95-95-4	Trichlorophenol, 2,4,5-	No	0.0313938	8.0893×10^{-6}	1200	1.597	1597	0.00006623058053	197.45	1	0.0362	69
88-06-2	Trichlorophenol, 2,4,6-	No	0.0313948	8.0896×10^{-6}	800	0.381	381	0.00010629599345	197.45	1	0.0346	69
93-76-5	Trichlorophenoxyacetic Acid, 2,4,5-	No	0.0288853	7.7627×10^{-6}	278	0.107	107	$3.5486508585445 \times 10^{-7}$	255.49	0.9	0.00914	153
93-72-1	Trichlorophenoxypropionic acid, -2,4,5	No	0.0233585	5.9194×10^{-6}	71	0.1753	175.3	$3.7040065412919 \times 10^{-7}$	269.51	0.9	0.0161	181.6

CAS Number[1]	Compound	VOC	D_{ia} (cm^2/s)	D_{iw} (cm^2/s)	Solubility (mg/L)	K_d (cm^3/g)	K_{oc} (cm^3/g)	H' (unitless)	MW (g/mol)	FA	Kp (cm/h)	Melting Point (°C)
96-18-4	Trichloropropane, 1,2,3-	Yes	0.0574661	9.2411×10^{-6}	1750	0.1158	115.8	0.01402289452166	147.43	1	0.00752	-14.7
95-63-6	Trimethylbenzene, 1,2,4-	Yes	0.0606754	7.9209×10^{-6}	57	0.6143	614.3	0.25183973834832	120.2	1	0.0857	-43.8
108-67-8	Trimethylbenzene, 1,3,5-	Yes	0.0602254	7.843×10^{-6}	48.2	0.6021	602.1	0.3585445625511	120.2	1	0.0621	-44.7
688-73-3	Tri-n-butyltin	Yes	0.0214738	5.351×10^{-6}	0.0073	8.091	8091	62.142273098937	291.05	0.9	0.0193	28.89
99-35-4	Trinitrobenzene, 1,3,5-	No	0.0289685	7.6882×10^{-6}	278	1.683	1683	$2.6573998364677 \times 10^{-7}$	213.11	1	0.000607	121.5
118-96-7	Trinitrotoluene, 2,4,6-	No	0.0295093	7.9182×10^{-6}	115	2.812	2812	$8.5036794766966 \times 10^{-7}$	227.13	1	0.000963	80.1
7440-62-2	Vanadium and Compounds	No	-	-	-	1000	-	-	50.94	1	0.001	1910
108-05-4	Vinyl Acetate	Yes	0.0849016	0.00001	20000	0.005583	5.583	0.02089125102207	86.091	1	0.00157	-93.2
75-01-4	Vinyl Chloride	Yes	0.1071202	0.000012	8800	0.02173	21.73	1.13654946852003	62.499	1	0.00838	-153.7
1330-20-7	Xylenes	Yes	0.0685148	8.4641×10^{-6}	106	0.3829	382.9	0.2710547833197	106.17	1	0.05	-25.2
7440-66-6	Zinc and Compounds	No	-	-	-	62	-	-	65.37	1	0.0006	419.5

Sources for the parameters listed in this table were obtained using the chemical parameter hierarchy found in Section 1.0 of this document.

[1] "CAS Number" means the Chemical Abstract Service (CAS) registry number uniquely assigned to chemicals by the American Chemical Society and recorded in the CAS Registry System

[2] "c" means carcinogenic, "nc" means noncarcinogenic, and "m" means mutagenic

[3] Hydrazine Kd value is taken from the National Institute of Health's Toxic Substances Databank

[4] Methyl mercury Kd value is taken from U.S. EPA. 1997 Mercury Study Report to Congress. EPA-452/R-97-005. Office of Air Quality Planning and Standards and Office of Research and Development. December

[5] PFOS and PFOA Koc values are taken from Higgins C and Luthy R. (2006) Sorption of Perfluorinated Surfactants on Sediments. Environ Sci Technol. 40(23):7251–7256.

Appendix B – Table 8 - Standard Default Factors for Non-Petroleum Organic and Inorganic Contaminants

Symbol	Definition (units)	Default	Reference(s)
A	Dispersion constant (unitless)	Arctic Zone = 7.1414 Under 40" Zone = 16.2302 Over 40" Zone = 14.2253	U.S. EPA 2002 Harding Lawson Associates
AF	Attenuation factor (unitless)	4	Professional judgment
AF_{0-2}	Skin adherence factor – age segment 0 – 2 years old (mg/cm^2)	0.2	U.S. EPA 2004
AF_{2-6}	Skin adherence factor – age segment 2 – 6 years old (mg/cm^2)	0.2	U.S. EPA 2004
AF_{6-16}	Skin adherence factor – age segment 6 – 16 years old (mg/cm^2)	0.07	U.S. EPA 2004
AF_{16-26}	Skin adherence factor – age segment 16 – 26 years old (mg/cm^2)	0.07	U.S. EPA 2004
AF_{iw}	Skin adherence factor – indoor worker (mg/cm^2)	0.12	U.S. EPA 2011
AF_{ow}	Skin adherence factor – indoor worker (mg/cm^2)	0.12	U.S. EPA 2011
AF_{ressa}	Skin adherence factor – resident soil adult (mg/cm^2)	0.07	U.S. EPA 2004
AF_{ressc}	Skin adherence factor – resident soil child (mg/cm^2)	0.2	U.S. EPA 2004
A_s	Areal extent of the site or contamination (acres)	0.5	U.S. EPA 2002
AT_{iw}	Averaging time – indoor worker (days)	365 x ED_{iws} = 9125	U.S. EPA 1989
AT_{ow}	Averaging time – outdoor worker (days)	365 x ED_{ows} =9125	U.S. EPA 1989
AT_{ress}	Averaging time – resident soil (days)	365 x LT = 25550	U.S. EPA 1989
AT_{ressa}	Averaging time – resident soil adult (days)	365 x ED_{ress} = 9490	U.S. EPA 1989
AT_{ressc}	Averaging time – resident soil child (days)	365 x ED_{ressc} = 2190	U.S. EPA 1989
AT_{resw}	Averaging time – resident groundwater (days)	365 x LT = 25550	U.S. EPA 1989
AT_{reswa}	Averaging time – resident groundwater adult (days)	365 x ED_{reswa} = 9490	U.S. EPA 1989
AT_{reswc}	Averaging time – resident groundwater child (days)	365 x ED_{reswc} = 2190	U.S. EPA 1989
B	Dispersion constant (unitless)	Arctic Zone = 31.1794 Under 40" Zone = 18.7762 Over 40" Zone = 18.8366	U.S. EPA 2002 Harding Lawson Associates
BW_{0-2}	Body weight – age segment 0 – 2 years old (kg)	15	U.S. EPA 2011
BW_{2-6}	Body weight – age segment 2 – 6 years old (kg)	15	U.S. EPA 2011

Symbol	Definition (units)	Default	Reference(s)
BW_{6-16}	Body weight – age segment 6 – 16 years old (kg)	80	U.S. EPA 2011
BW_{16-26}	Body weight – age segment 16 – 26 years old (kg)	80	U.S. EPA 2011
BW_{iw}	Body weight – indoor worker (kg)	80	U.S. EPA 2011
BW_{ow}	Body weight – outdoor worker (kg)	80	U.S. EPA 2011
BW_{ressa}	Body weight –adult (kg)	80	U.S. EPA 2011
BW_{ressc}	Body weight –child (kg)	15	U.S. EPA 2011
BW_{reswa}	Body weight –adult (kg)	80	U.S. EPA 2011
BW_{reswc}	Body weight –child (kg)	15	U.S. EPA 2011
C	Dispersion constant (unitless)	Arctic Zone = 382.6078 Under 40" Zone = 216.108 Over 40" Zone = 218.1845	U.S. EPA 2002 Harding Lawson Associates
d	Mixing zone depth (m)	5.5	U.S. EPA. 2002
d_a	Aquifer thickness (m)	10	U.S. EPA. 2002
d_s	Depth of source (m)	5.5	U.S. EPA. 2002
DAF	Dilution attenuation factor (unitless)	13.2	U.S. EPA. 2002
DF	Dilution factor (unitless)	3.3	Professional judgment
$DFSM_{res-adj}$	Mutagenic dermal contact factor – resident soil age-adjusted (mg/kg)	Arctic Zone = 244720 Under 40" Zone = 330372 Over 40" Zone = 403788	Calculated using the age adjusted intake factors equation
$DFS_{res-adj}$	Dermal contact factor – resident soil age-adjusted (mg/kg)	Arctic Zone = 59080 Under 40" Zone = 79758 Over 40" Zone =97482	Calculated using the age adjusted intake factors equation
$DFWM_{res-adj}$	Mutagenic dermal contact factor – resident groundwater age-adjusted (cm^2 - event/kg)	8191633	Calculated using the age adjusted intake factors equation
$DFW_{res-adj}$	Dermal contact factor – resident groundwater age-adjusted (cm^2 - event/kg)	2610650	Calculated using the age adjusted intake factors equation
ED_{0-2}	Exposure duration – age segment 0 – 2 years old (years)	2	Time Frame
ED_{2-6}	Exposure duration – age segment 2 – 6 years old (years)	4	Time Frame
ED_{6-16}	Exposure duration – age segment 6 – 16 years old (years)	10	Time Frame

Symbol	Definition (units)	Default	Reference(s)
ED_{16-26}	Exposure duration – age segment 16 – 26 years old (years)	10	Time Frame
ED_{iw}	Exposure duration – indoor worker (years)	25	U.S. EPA 1991a
ED_{ow}	Exposure duration – outdoor worker (years)	25	U.S. EPA 1991a
ED_{ress}	Exposure duration – resident soil (years)	26	EPA 2011
ED_{ressa}	Exposure duration – resident soil adult (years)	20	U.S. EPA 1991a
ED_{ressc}	Exposure duration – resident soil child (years)	6	U.S. EPA 1991a
ED_{resw}	Exposure duration – resident groundwater (years)	26	EPA 2011
ED_{reswa}	Exposure duration – resident groundwater adult (years)	20	U.S. EPA 1991a
ED_{reswc}	Exposure duration – resident groundwater child (years)	6	U.S. EPA 1991a
EF_{0-2}	Exposure frequency – age segment 0 – 2 years old (days/year)	Arctic Zone = 200 Under 40" Zone = 270 Over 40" Zone = 330 Migration to Groundwater = 350 Groundwater = 350	Harding Lawson Associates
EF_{2-6}	Exposure frequency – age segment 2 – 6 years old (days/year)	Arctic Zone = 200 Under 40" Zone = 270 Over 40" Zone = 330 Migration to Groundwater = 350 Groundwater = 350	Harding Lawson Associates
EF_{6-16}	Exposure frequency – age segment 6 – 16 years old (days/year)	Arctic Zone = 200 Under 40" Zone = 270 Over 40" Zone = 330 Migration to Groundwater = 350 Groundwater = 350	Harding Lawson Associates
EF_{16-26}	Exposure frequency – age segment 16 – 26 years old (days/year)	Arctic Zone = 200 Under 40" Zone = 270 Over 40" Zone = 330 Migration to Groundwater = 350 Groundwater = 350	Harding Lawson Associates
EF_{iws}	Exposure frequency – indoor worker soil (days/year)	Arctic Zone = 200 Under 40" Zone = 250 Over 40" Zone = 250	Harding Lawson Associates

Symbol	Definition (units)	Default	Reference(s)
EF_{ows}	Exposure frequency – outdoor worker soil (days/year)	Arctic Zone = 200 Under 40" Zone = 250 Over 40" Zone = 250	Harding Lawson Associates
EF_{ress}	Exposure frequency - resident soil (days/year)	Arctic Zone = 200 Under 40" Zone = 270 Over 40" Zone = 330	Harding Lawson Associates
EF_{ressa}	Exposure frequency – resident soil adult (days/year)	Arctic Zone = 200 Under 40" Zone = 270 Over 40" Zone = 330	Harding Lawson Associates
EF_{ressc}	Exposure frequency – resident soil child (days/year)	Arctic Zone = 200 Under 40" Zone = 270 Over 40" Zone = 330	Harding Lawson Associates
EF_{resw}	Exposure frequency – resident groundwater (days/year)	350	U.S. EPA 1991a
EF_{reswa}	Exposure frequency – resident groundwater adult (days/year)	350	U.S. EPA 1991a
EF_{reswc}	Exposure frequency – resident groundwater child (days/year)	350	U.S. EPA 1991a
ET_{0-2}	Exposure time - age segment 0 – 2 years old (hours/day)	24	The whole day
ET_{2-6}	Exposure time - age segment 2 – 6 years old (hours/day)	24	The whole day
ET_{6-16}	Exposure time - age segment 6 – 16 years old (hours/day)	24	The whole day
ET_{16-26}	Exposure time - age segment 16 – 26 years old (hours/day)	24	The whole day
ET_{0-2}^{der}	Dermal exposure time - age segment 0 – 2 years old (hours/event)	0.54	U.S. EPA 2011
ET_{2-6}^{der}	Dermal exposure time - age segment 2 – 6 years old (hours/event)	0.54	U.S. EPA 2011
ET_{6-16}^{der}	Dermal exposure time - age segment 6 – 16 years old (hours/event)	0.71	U.S. EPA 2011
ET_{16-26}^{der}	Dermal exposure time - age segment 16 – 26 years old (hours/event)	0.71	U.S. EPA 2011
ET_{0-2}^{inh}	Inhalation exposure time - age segment 0 – 2 years old (hours/event)	24	The whole day
ET_{2-6}^{inh}	Inhalation exposure time - age segment 2 – 6 years old (hours/event)	24	The whole day
ET_{6-16}^{inh}	Inhalation exposure time - age segment 6 – 16 years old (hours/event)	24	The whole day
ET_{16-26}^{inh}	Inhalation exposure time - age segment 16 – 26 years old (hours/event)	24	The whole day
ET_{ress}	Exposure time - resident soil (hours/day)	24	The whole day
ET_{ressa}	Exposure time – resident soil adult (hours/day)	24	The whole day
ET_{ressc}	Exposure time – resident soil child (hours/day)	24	The whole day

Symbol	Definition (units)	Default	Reference(s)
ET_{resw}	Exposure time – resident groundwater (hours/day)	24	The whole day
ET_{resw}^{inh}	Inhalation exposure time – resident groundwater (hours/day)	24	The whole day
ET_{reswa}^{der}	Dermal exposure time – resident groundwater adult (hours/event)	0.71	U.S. EPA 2011
ET_{reswa}^{inh}	Inhalation exposure time – resident groundwater adult (hours/event)	24	The whole day
ET_{reswc}^{der}	Dermal exposure time – resident groundwater child (hours/event)	0.54	U.S. EPA 2011
ET_{reswc}^{inh}	Inhalation exposure time – resident groundwater child (hours/event)	24	The whole day
$ET_{resw\text{-}adj}^{der}$	Dermal exposure time – resident groundwater age-adjusted (hours/day)	0.67077	U.S. EPA 2011
$ET_{resw\text{-}adj}^{inh}$	Inhalation exposure time – resident groundwater age-adjusted (hours/day)	24	The whole day
$ET_{resw\text{-}madj}$	Mutagenic exposure time – resident groundwater age-adjusted (hours/day)	0.67077	U.S. EPA 2011
$EV_{0\text{-}2}$	Exposure events – age segment 0 – 2 years old (events/day)	1	U.S. EPA 2011
$EV_{2\text{-}6}$	Exposure events – age segment 2 – 6 years old (events/day)	1	U.S. EPA 2011
$EV_{6\text{-}16}$	Exposure events – age segment 6 – 16 years old (events/day)	1	U.S. EPA 2011
$EV_{16\text{-}26}$	Exposure events – age segment 16 – 26 years old (events/day)	1	U.S. EPA 2011
EV_{reswa}	Exposure events – resident groundwater adult (events/day)	1	U.S. EPA 2011
EV_{reswc}	Exposure events – resident groundwater child (events/day)	1	U.S. EPA 2011
F(x)	Function dependent on u_m / u_t (unitless)	Arctic Zone = 0.57 Under 40" Zone = 0.194 Over 40" Zone = 0.0616	U.S. EPA 1996a
f_{oc}	Fraction organic carbon in soil (g/g)	0.001 (0.1%)	U.S. EPA. 2002
I	Infiltration rate (m/year)	0.13	U.S. EPA. 2002

Symbol	Definition (units)	Default	Reference(s)
i	Hydraulic gradient (m/m)	0.002	U.S. EPA. 2002
$IFSM_{res-adj}$	Mutagenic soil ingestion rate – resident age-adjusted (mg/kg)	Arctic Zone = 95333 Under 40" Zone = 128700 Over 40" Zone = 157300	Calculated using the age adjusted intake factors equation
$IFS_{res-adj}$	Soil ingestion rate – resident age-adjusted (mg/kg)	Arctic Zone = 21000 Under 40" Zone = 28350 Over 40" Zone = 34650	Calculated using the age adjusted intake factors equation
$IFWM_{res-adj}$	Mutagenic groundwater ingestion rate – resident age-adjusted (L/kg)	1019.9	Calculated using the age adjusted intake factors equation
$IFW_{res-adj}$	Groundwater ingestion rate – resident age-adjusted (L/kg)	327.95	Calculated using the age adjusted intake factors equation
IRS_{0-2}	Soil ingestion rate - age-segment 0 – 2 years old (mg/day)	200	U.S. EPA 1991a (pg. 15)
IRS_{2-6}	Soil ingestion rate - age-segment 2 – 6 years old (mg/day)	200	U.S. EPA 1991a (
IRS_{6-16}	Soil ingestion rate - age-segment 6 – 16 years old (mg/day)	100	U.S. EPA 1991a
IRS_{16-26}	Soil ingestion rate - age-segment 16 – 26 years old (mg/day)	100	U.S. EPA 1991a
IRS_{iw}	Soil ingestion rate – indoor worker (mg/day)	50	U.S. EPA 1991a
IRS_{ow}	Soil ingestion rate – outdoor worker (mg/day)	100	U.S. EPA 1991a
IRS_{ressa}	Soil ingestion rate – resident soil adult (mg/day)	100	U.S. EPA 1991a
IRS_{ressc}	Soil ingestion rate – resident soil child (mg/day)	200	U.S. EPA 1991a
IRW_{0-2}	Resident groundwater ingestion rate - age-segment 0 – 2 years old (L/day)	0.78	U.S. EPA 2011
IRW_{2-6}	Resident groundwater ingestion rate - age-segment 2 – 6 years old (L/day)	0.78	U.S. EPA 2011
IRW_{6-16}	Resident groundwater ingestion rate - age-segment 6 – 16 years old (L/day)	2.5	U.S. EPA 2011
IRW_{16-26}	Resident groundwater ingestion rate - age-segment 16 – 26 years old (L/day)	2.5	U.S. EPA 2011
IRW_{iw}	Groundwater ingestion rate – indoor worker (L/day)	2.5	U.S. EPA 2011
IRW_{ow}	Groundwater ingestion rate – outdoor worker (L/day)	2.5	U.S. EPA 2011
IRW_{reswa}	Groundwater ingestion rate – resident groundwater adult (L/day)	2.5	U.S. EPA 2011
IRW_{reswc}	Groundwater ingestion rate – resident groundwater child (L/day)	0.78	U.S. EPA 2011

Symbol	Definition (units)	Default	Reference(s)
K	Andelman volatilization factor (L/m^3)	0.5	U.S. EPA 1991b
K	Aquifer hydraulic conductivity (m/year)	876	U.S. EPA. 2002
L	Source length parallel to ground water flow (m)	32	U.S. EPA. 2002
LT	Lifetime (years)	70	U.S. EPA 1989
n	Total soil porosity(L_{pore}/L_{soil})	= $1-(\varrho_b/\varrho_s)$ = 0.43396	U.S. EPA. 2002
PEF_w	Particulate emission factor (m^3/kg)	Arctic Zone = 1.47×10^9 Under 40" Zone = 1.36×10^9 Over 40" Zone = 1.28×10^9	Determined in the calculations
Q/C	Inverse of the mean concentration at the center of a 0.5-acre-square source (g/m^2-s per kg/m^3)	Arctic Zone = 101.5958 Under 40" Zone = 93.7736 Over 40" Zone = 81.7066	Harding Lawson Associates
SA_{0-2}	Skin surface area – resident age segment 0 – 2 years old (cm^2)	Soil = 2373 Migration to Groundwater = 6365 Groundwater = 6365	U.S. EPA 2011
SA_{2-6}	Skin surface area – resident age segment 2 – 6 years old (cm^2)	Soil = 2373 Migration to Groundwater = 6365 Groundwater = 6365	U.S. EPA 2011
SA_{6-16}	Skin surface area – resident age segment 6 – 16 years (cm^2)	Soil = 6032 Migration to Groundwater = 19652 Groundwater = 20900	U.S. EPA 2011
SA_{16-26}	Skin surface area – resident age segment 16 – 26 years (cm^2)	Soil = 6032 Migration to Groundwater = 19652 Groundwater = 20900	U.S. EPA 2011
SA_{iw}	Skin surface area – indoor worker (cm^2)	3527	US EPA 2011
SA_{ow}	Skin surface area – outdoor worker (cm^2)	3527	US EPA 2011
SA_{ressa}	Skin surface area – resident soil adult (cm^2)	6032	U.S. EPA 2011
SA_{ressc}	Skin surface area – resident soil child (cm^2)	2373	U.S. EPA 2011
SA_{reswa}	Skin surface area – resident groundwater adult (cm^2)	19652	U.S. EPA 2011
SA_{reswc}	Skin surface area – resident groundwater child (cm^2)	6365	U.S. EPA 2011
T	Exposure interval (s)	819936000	U.S. EPA. 2002
THQ	Target hazard quotient	1.0	18 AAC 75.990(50)

Symbol	Definition (units)	Default	Reference(s)
TR	Target risk	1×10^{-5}	Determined in this calculator
U_m	Mean annual wind speed (m/s)	Arctic Zone = 5.77 Under 40" Zone = 4.69 Over 40" Zone = 4.07	U.S. EPA 1996a
U_t	Equivalent threshold value of wind speed at 7m (m/s)	11.32	U.S. EPA 1996a
V	Fraction of vegetative cover (unitless)	0.5	U.S. EPA 1996a
θ_a	Air-filled soil porosity (L_{air}/L_{soil})	$= n-\theta_w = 0.28396$	U.S. EPA. 2002
θ_w	Water-filled soil porosity (L_{water}/L_{soil})	0.15	U.S. EPA. 2002
ϱ_b	Dry soil bulk density (kg/L)	1.5	U.S. EPA. 2002
ϱ_s	Soil particle density (kg/L)	2.65	U.S. EPA. 2002

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